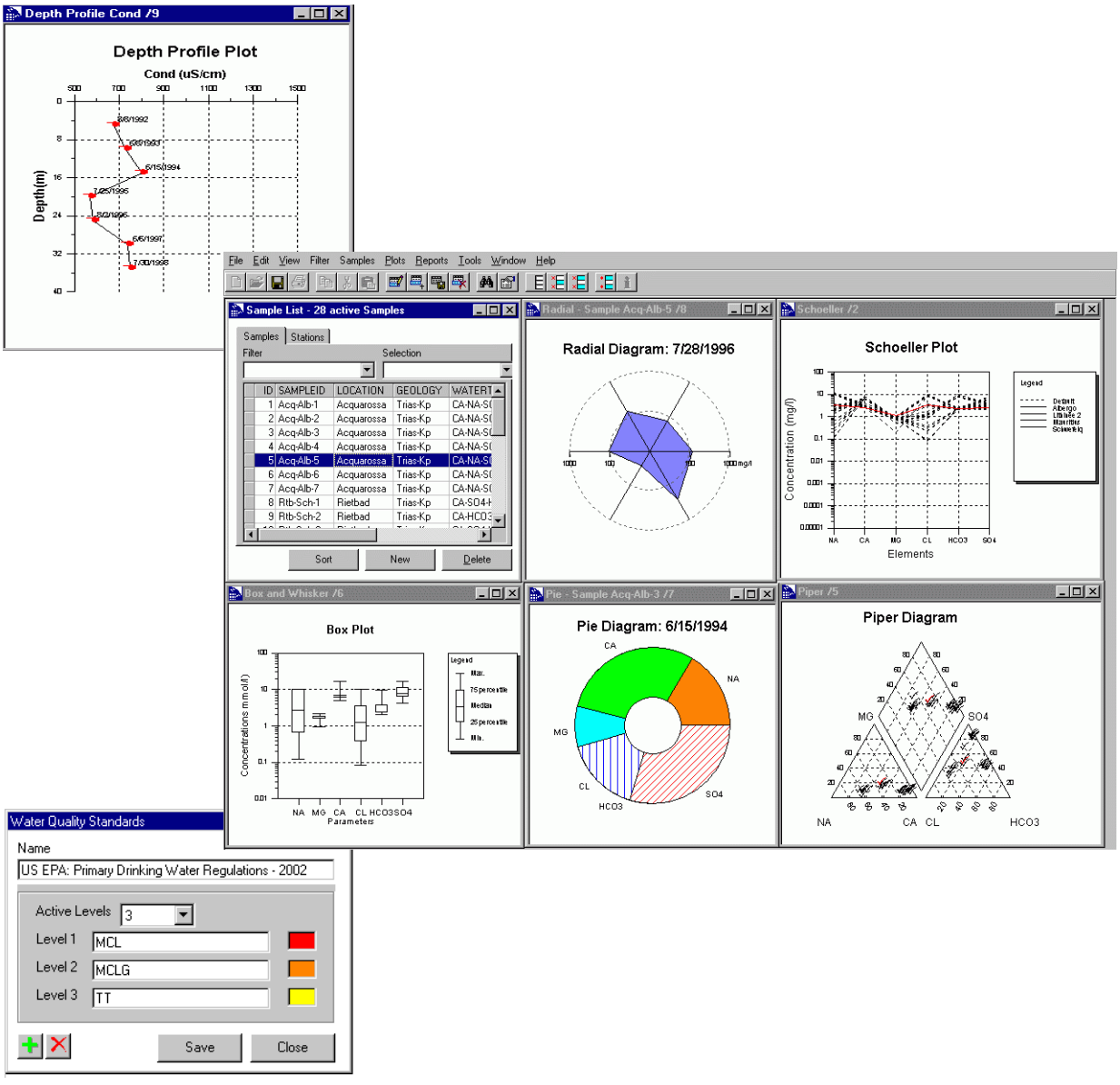
AquaChem v.4.0

User's Manual

Water Quality Data Analysis, Plotting, and Modeling



Co-Developed by Lukas Calmbach and Waterloo Hydrogeologic, Inc.

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Preface

How to Contact Waterloo Hydrogeologic, Inc.

If after reading this manual and using AquaChem, you would like to contact Waterloo Hydrogeologic with comments or suggestions, or if you need technical assistance, you can reach us at:

Waterloo Hydrogeologic Inc.
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Waterloo, Ontario,
CANADA, N2L 5J2

Phone: +1 (519) 746 1798
Fax: +1 (519) 885 5262
E-mail: techsupport@flowpath.com
Web: www.waterloohydrogeologic.com

Obtaining Technical Support

To help us handle your technical support questions as quickly as possible, please have the following information ready before you call, or include it in a detailed technical support e-mail:

- A complete description of the problem including a summary of key strokes and program event (or a screen capture showing the error message, where applicable)
- Product name and version number
- Product serial number
- Computer make and model number
- Operating system and version number
- Total free RAM
- Number of free bytes on your hard disk
- Software Installation directory
- Directory location for your current project files

You may send us your questions via e-mail, fax, or call one of our technical support specialists. Please allow up to two business days for a response. Technical support is available 9:00 am to 5:00 pm EST Monday to Friday (excluding Canadian holidays).

Waterloo Hydrogeologic, Inc. Training and Consulting

Waterloo Hydrogeologic strives to offer the most useful, practical, high quality training in hydrogeologic modeling in the industry. Training courses are designed to provide a rapid introduction to essential knowledge and skills, and create a basis for further professional development and real-world practice. Open enrollment courses are offered worldwide each year. For the current schedule of courses, visit: www.waterloohydrogeologic.com or e-mail us at:

training@flowpath.com.

Waterloo Hydrogeologic also offers expert consulting and reviewing services for all numerical modeling projects concerning groundwater flow and solute transport. For further information, please contact us at:

consulting@flowpath.com.

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We also develop and distribute a number of other useful software products for the groundwater professionals, all designed to increase your efficiency and enhance your technical capability, including:

- Visual MODFLOW Pro
- Visual MODFLOW 3D-Explorer
- WinPEST
- RISC WorkBench
- Visual PEST
- Visual Groundwater
- WHI UnSatSuite
- Visual HELP
- Remediation ToolKit
- Aquifer Test Pro
- FLOWPATH II

Visual MODFLOW Pro

...is the largest time-saving breakthrough since the release of MODFLOW for building, calibrating, and analyzing groundwater flow and contaminant transport models. Setting the environmental industry standard, Visual MODFLOW Pro is a pre- and post-processor for MODFLOW, MODPATH, and MT3D/RT3D. Visual MODFLOW Pro is the complete package for groundwater modeling and includes the Visual MODFLOW 3D-Explorer and WinPEST (see descriptions below).

Visual MODFLOW 3D-Explorer

...is a built-in 3D visualization system for displaying and animating Visual MODFLOW models using state-of-the-art 3D graphics technology. The advanced visualization capabilities of the Visual MODFLOW 3D-Explorer provide you with all the tools you need to create impressive and informative 3D representations of your modeling data using vibrant colors and high-resolution graphics.

WinPEST

...is exclusively designed for Visual MODFLOW Pro to help reduce the tedious hours spent calibrating model results to observations found in the field. WinPEST is completely integrated within Visual MODFLOW Pro and offers a variety of benefits unparalleled in other calibration packages.

RISC WorkBench

...is an easy-to-use software package designed for performing fate and transport modeling and human health risk assessments for contaminated sites. Following standard procedures outlined by the U.S. EPA,

the RISC WorkBench calculates exposure assessment, toxicity assessment, and risk assessment. RISC WorkBench also includes a completely customizable database for common environmental parameters used when conducting risk assessments.

Visual PEST

...combines the latest version of PEST2000 with the graphical processing and display features of WinPEST for model-independent parameter estimation.

Visual Groundwater

...is the first software package to combine state-of-the-art graphical technology for 3D visualization and animation capabilities with an easy-to-use graphical interface designed specifically for environmental project applications.

WHI UnSat Suite

...is a fully-integrated software package for modeling 1D unsaturated zone flow and contaminant transport using the industry standard numerical modeling codes - all run under one tightly integrated interface.

Visual HELP

...is the most advanced hydrological modeling environment available for designing landfills, predicting leachate mounding and evaluating potential leachate seepage to the groundwater table.

Remediation ToolKit

...provides an integrated data management, visualization, trend analysis, and modeling platform for evaluating the effectiveness of Monitored Natural Attenuation. The Remediation ToolKit combines 3 different software applications (BioTrends, SEQUENCE and BioTracker) into one integrated solution for evaluating, visualizing and modeling natural attenuation processes.

AquiferTest Pro

...is the most complete and easy-to-use software package for graphical analysis and reporting of pumping test and slug test data analysis. The software comes with a comprehensive selection of built-in solution methods for estimating transmissivity, hydraulic conductivity, and storage properties for confined, unconfined, leaky and fractured rock aquifers. The Pro version now includes new forward/predictive solutions, which allow you to predict drawdown under a new set of stresses, including the influence of multiple pumping wells, barrier/recharge boundaries, and well effects.

Flowpath II

...is a popular two-dimensional, steady-state, groundwater flow, pathline, and contaminant transport model that computes hydraulic heads, pathlines, travel times, velocities, water balances, and contaminant concentrations (approved by the US EPA and recommended by the UK Environmental Agency).

At Waterloo Hydrogeologic, we are continually developing new modeling and visualization applications for the environmental professionals. For more information, please contact us.

Table of Contents

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Introduction to AquaChem

AquaChem is a software package developed specifically for graphical and numerical analysis and modeling of water quality data. It features a fully customizable database of physical and chemical parameters and it provides a comprehensive selection of analysis tools, calculations and graphs for interpreting water quality data.

AquaChem's data analysis capabilities cover a wide range of functionalities and calculations including unit conversions, charge balances, sample comparison and mixing, statistical summaries, trend analysis, and much more. AquaChem also has a customizable database of water quality standards with up to three different action levels for each parameter. Any samples exceeding the selected standard are automatically highlighted with the appropriate action level color for easily identifying and qualifying potential problems.

These powerful analytical capabilities are complemented by a comprehensive selection of commonly used plotting techniques to represent the chemical characteristics of water quality data. The plot types available in AquaChem include:

- Correlation plots: X-Y Scatter, Ludwig-Langelier, and Wilcox
- Summary plots: Box and Whisker, Frequency Histogram, and Schoeller
- Trilinear plots: Piper, Durov, Ternary, and Giggenbach
- Time-Series plot
- Geothermometer plot
- Sample plots: Radial, Stiff, and Pie
- Thematic Map plots: Bubble, Pie, Radial and Stiff plots at sample locations

Each of these plots provides a unique interpretation of the many complex interactions between the groundwater and aquifer materials, and identifies important data trends and groupings.

In addition, AquaChem features a built-in link to the popular geochemical modeling program PHREEQC for calculating equilibrium concentrations (or activities) of chemical species in solution and saturation indices of solid phases in equilibrium with a solution. For more advanced simulations, you may link to PHREEQC-I or PHREEQC for Windows, and use your AquaChem samples as input solutions for these modeling utilities.

Once you start using AquaChem, you will see that it is truly one of the most powerful tools available for interpretation, analysis and modeling of simple or complex water quality data sets.

New Features in Version 4.0

Database Format

In previous versions of AquaChem, the database was maintained as a "flat" table where all the information for each water sample was stored in a single record (row) of the table. Although this format is very simple and easy to understand, it is very inefficient in terms of data storage and data access. If multiple samples were taken from the same location over the course of many years, this required the user to continually re-enter and store the same location information for each sample record. This made the database unnecessarily large, slowed the execution of database queries, and made it difficult to ensure consistency of the data.

AquaChem v.4.0 leverages the efficiencies of a MS Access relational database structure with a logical '**Station Centric**' hierarchy. A **Station** is defined as a unique spatial location where a water **Sample** is collected. The stations maintain a Parent-Child relationship with the samples, whereby each station is a Parent and each sample is a Child. While a station may 'own' many samples, each sample may only 'belong' to a single station. The information for each unique station is stored in a table where each column (field) represents an attribute of the station, and each row (record) stores the information for each field. Please see the list of Mandatory Station Parameters in Chapter 3 for more details.

The information for the samples is stored separately from the stations table, but each unique sample is necessarily linked to the stations table, since each sample must be owned by one station. The information required for each sample is broken into three separate groups of data: Sample Description, Measured Parameters, and Modeled Parameters. Please see the list of Mandatory Sample Parameters in Chapter 3 for more details.

This hierarchical database structure provides improvements in performance, more flexibility for customizing parameters, and many built-in data integrity rules.

Importing Data

In most situations, the data used by AquaChem will need to be imported from a file provided by a client, a lab, or generated by some other software application. This data may be provided in a number of different formats which do not likely coincide exactly with the database structure used by AquaChem. Furthermore, the chemical names used in the source file may be different than the field names used in AquaChem. As a result, AquaChem v.4.0 provides an option to choose from a selection of data formats, and to

use the CAS Registry Number to automatically map the source file chemical names to the AquaChem field names.

Filtering Data

When working with large databases containing hundreds or thousands of water quality samples, it is necessary to be able to quickly and easily filter the sample records to show only samples satisfying a user-defined criteria. AquaChem v.4.0 allows you to easily create, apply and save an unlimited number of customized filters (ex. Na > 100 mg/L). Any one of these filters can be selected and applied to the sample list using just two mouse clicks.

Plots

The new plotting options include:

- Depth Profile, Box & Whisker Plot, and Wilcox plots.
- True-type AquaChem symbol fonts for higher quality display and printing
- Automatically assign symbols to samples based on a selected descriptive parameter (i.e. location, project number, date, etc.).
- Multiple symbol groups that allow you to create, store and recall different symbol configurations for the list of samples.
- Customized auto-titling of Pie, Stiff, and Radial plots (ex. create a default title containing the fields [Sample ID] and [Sample Date] for each sample plot).
- More options for customizing the appearance of the plot legends.

Utility Tools

Several new Calculator utility tools have been added to AquaChem v.4.0 to provide convenient access to some of the calculations and conversions you may wish to evaluate during the course of working on your projects. These utility tools include:

- Unit Calculator: Converts values from one measurement unit to another for most common units categories.
- Formula Weight Calculator: Calculates the formula weight of virtually any organic or inorganic chemical.
- Species Converter: Converts any species into a different form. This is useful to express a measured amount of a parameter as a different aqueous species when expressed in mg/L.
- Volume Concentration Converter: Converts volume concentration (ppm) of a specified chemical formula to mass concentration (mg/m3).
- Special Units Converter: Converts values from one measurement unit to another for measurement units such as pe - Eh, Alkalinity - HCO3, and Conductivity (us) - Resistivity (Ohm/cm).

- Decay Calculator: Calculates the concentration of a chemical after a period of time subject to a specified decay rate, or calculates the time required for a chemical to reach a specified concentration subject to specified decay rate.

Water Quality Standards

The ability to compare the water quality data to selected water quality standards is an important process in any water quality analysis. AquaChem v.4.0 now allows you to create and manage multiple sets of water quality standards with up to three different action levels for each parameter. Three popular water quality standards are included with AquaChem (WHO, USEPA, and CCME) while any other standards are easily imported. This new version also provides an option to automatically highlight exceedences (with different colors for each action level) while viewing individual sample details or in tabular views, and you can easily switch from one standard to another at any time during the project.

Water Quality Modeling

AquaChem v.4.0 makes it easier than ever to quickly utilize the most basic functionality of the popular USGS PHREEQC program directly from the AquaChem interface. Now, with just one click of the mouse, you can use PHREEQC to calculate the saturation indices or activities for selected water quality samples and store the results back into the AquaChem sample database record.

For more complex water quality modeling scenarios, AquaChem v.4.0 provides a link to one of the popular public domain graphical interfaces for PHREEQC available from the USGS Water Resources Software web site (the user can choose to link to either the USGS PHREEQC-Interactive program, or to the PHREEQC for Windows program development by Vincent Post). In each case, AquaChem creates one or more solutions using selected samples from the AquaChem database and passes these to the PHREEQC graphical interface program.

Reporting Options

AquaChem v.4.0 has also improved many of the reporting features to give you the ability to create attractive printed reports directly from AquaChem:

- Custom Report Designer allows you to create sample reports containing any set of selected parameters and to format the organization and presentation of the results.
- Template Designer has been improved to make it easier to create customized page layouts for printed Reports and Plots.
- Plot Print Options have been improved to make it easier to select and customize the arrangement of plots on the page.

1.1 Installing AquaChem

System Requirements

To run **AquaChem** you require the following minimum system configuration:

- A CD-ROM drive for software installation
- A hard drive, with at least 35 MB free space
- A local or network printer installed
- A Pentium processor or better, with 32 MB RAM
- Windows 98/2000/XP, or Windows NT 4.0 with Service Pack 4 (or later) installed
- A Microsoft compatible mouse
- Minimum 1024 x 768 screen resolution
- Normal fonts

Installation

Stand Alone Installation

AquaChem is distributed on one CD-ROM. To install, please follow these directions:

- Place the CD into your CD-ROM drive and the initial installation screen should load automatically. Once loaded, an installation interface with several different tabs will be presented.
- Please take the time to explore the installation interface, as there is information concerning other Waterloo Hydrogeologic products, our worldwide distributors, technical support, consulting, training, and how to contact us.
- On the initial Installation tab, you may choose from the following two buttons: **AquaChem Installation** and **AquaChem User's Manual**
- The User's Manual button will display a PDF document of the manual, which requires the Adobe Reader to view. If you do not have the Adobe Reader, a link has been created in the interface to download the appropriate software.
- The Installation button will initiate the installation of AquaChem on your computer. AquaChem must be installed on your local hard disk in order to run. Follow the installation instructions, and read the on-screen directions carefully. You will be prompted to enter you name, company name and serial number. Please ensure that you enter your serial number exactly as is it appears on your CD case or invoice. Be sure to use capital letters and hyphens in the correct locations.
- If you select to install PHREEQC-I, this installation will commence following the AquaChem installation.
- Once the installation is completed, you must re-boot your computer for the system changes to take effect. After the installation is complete and your system

has re-booted, you should see the blue WHI icon on your Desktop screen labeled **AquaChem 4.0**. To start working with AquaChem, double-click on this icon.

To install the software from the CD-ROM without the aid of the installation interface, you can:

- Open Windows Explorer, and navigate to the CD-ROM drive
- Open the Installation folder
- Double-click the **Setup.exe** to initiate the installation

Follow the on-screen installation instructions, which will lead you through the install and subsequently produce a desktop icon for you.

Network Installation

You may also install and operate AquaChem over a local-area network. AquaChem supports a network server-client installation, whereby the server houses the program executable and database files, while each client houses all other supporting files (such as .DLL and .OCX files). AquaChem project database files may be saved in the server installation folder, in a sub-folder titled "Data" (which must be created by the user). Or, the files may be saved to any other folder on the server. The advantage of the network installation is that program can be run through a server machine, allowing for control of the licenses, and greater ease when updating the program.

Server

The server installation is simply a folder on the server, which contains the following program files: *Aquachem40.exe, Aquachem.mdb, Demo.aqc, Template.tpl, Template.37,* *.DXF, PHREEQC files (*phreeqc.exe*, *.dat), *AQCHelp.chm*, and supporting files data files.

Client

Each client machine contains all the supporting files required to run AquaChem. These include .DLL and .OCX files. Each client machine must have a drive mapped to the directory on the server machine which contains the AquaChem installation. At the end of the installation, each client needs a shortcut to the Aquachem40.exe on the server.

NOTE: AquaChem does not support multi-user simultaneous access of a project database. An Aquachem database may be opened, viewed, and modified by only one user at a time. Future versions of AquaChem will support this configuration.

PHREEQC-I Installation

During the installation, you will be prompted to install the USGS's PHREEQC-Interactive program. This program is a graphical interface for preparing and running complex geochemical modeling scenarios. AquaChem has a built-in link to the

PHREEQC-Interactive program that is capable of creating one or more solutions from the water quality samples in the AquaChem database.

If you choose not to install PHREEQC-Interactive during the initial installation, you may install this component later on. The PHREEQC-I installation is available in the PHREEQC folder on the installation CD-ROM; the file is named: **PhreeqcI28.exe**

PHREEQC for Windows Installation

AquaChem also supports a link to the PHREEQC for Windows program. This program is an alternative graphical interface that also allows for preparing and running advanced geochemical simulations. However, this program is not installed during the main AquaChem installation.

If you wish to install and use the PHREEQC for Windows program, the installation is available in the PHREEQC folder on the installation CD-ROM. The file is named: **psetup1510.exe**

These files are also available for download from the Waterloo Hydrogeologic ftp site:

ftp.flowpath.com

and from the USGS - PHREEQC home page:

http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

1.2 Uninstalling AquaChem

There may be instances where you will need to uninstall (remove) AquaChem from your system (i.e. if the software is to be transferred to another computer, or you need to reinstall on the current computer). To uninstall AquaChem:

- Locate the **Add/Remove Programs** option in your **Windows' Control Panel**.
- Select AquaChem 4.0 as the program to be removed
- Follow the on-screen instructions.
- Once you are finished, re-boot your system to ensure all system files are updated.

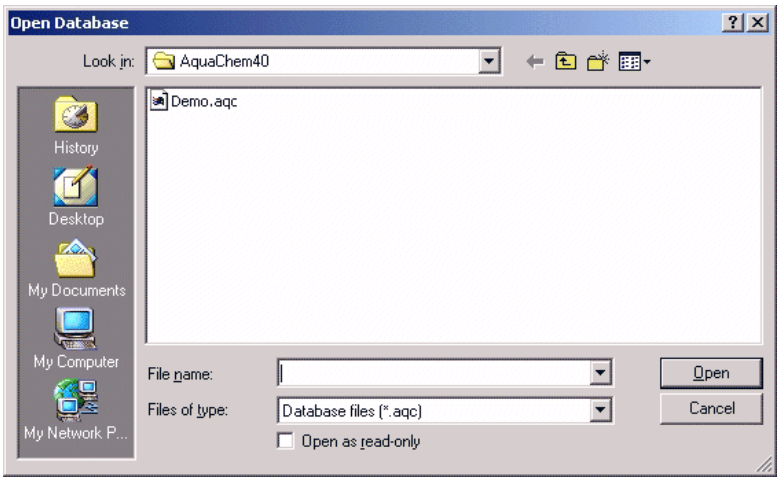
1.3 On-Line Help

This manual is supplied to you in two forms: as a printed book, and as an online help file. To view the online help version of this manual, select **Help > Contents**.

1.4 Starting AquaChem

To start AquaChem, you must have the program installed on your hard disk. If you have not yet installed AquaChem, please refer to the section, Installing AquaChem, which is described above. Otherwise start AquaChem by double-clicking on the desktop icon (as shown on the left-hand side), or by accessing **WHI Software/Aquachem 4.0** from your **Start > Programs** Windows menu.

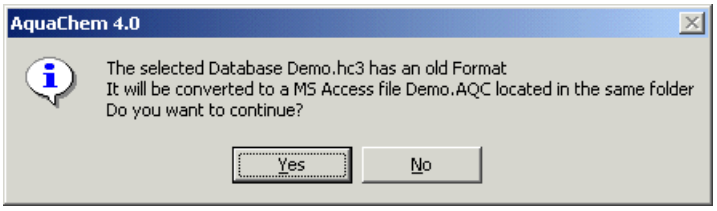
Upon starting AquaChem, the following **Open Database** dialogue will be displayed prompting you to select a valid AquaChem database.



Select the **Demo.aqc** file to open the demonstration database; to open a different database, browse to the appropriate folder. Otherwise, to create a new database click **[Cancel]** in this dialogue and select **File > New** from the main menu.

Opening Old Project Sets (from Version 3.7)

AquaChem version 4.0 is compatible with the previous version, version 3.7. To open a project set from v.3.7, use the **File > Open** command. You will be prompted with an **Open Database** dialogue. At the bottom of this dialogue, simply change the file type to **V3.7 Database (*.hc3)**. Then browse to the folder which contains your database from 3.7. Press **[Open]** and the following window will appear.



If you select **[Yes]**, the AquaChem database will be opened with a screen layout as shown on the next page, or if you select **[No]** then the option of opening the old project sets will be canceled.

Note that in AquaChem v 3.7, there are cases where there are duplicate parameter names (ex. “P” was used for p-value and Phosphorous). Since the database structure in v.4.0 requires a unique name and identifier for each parameter, a dataset with duplicate parameter names can cause problems. As such, the first time you open a project which contains duplicate parameter names, AquaChem will automatically read through all parameters first and prompt a message if a duplicate parameter is located. If this occurs, simply enter a new unique name for the duplicate parameter. In addition, your v.3.7 project may be missing some parameters which are required in a v.4.0 database. If so, you will be prompted to create these mandatory parameters in the v.4.0 project. Click **[Yes]** to create these mandatory parameters. After this, opening of the project should proceed successfully.

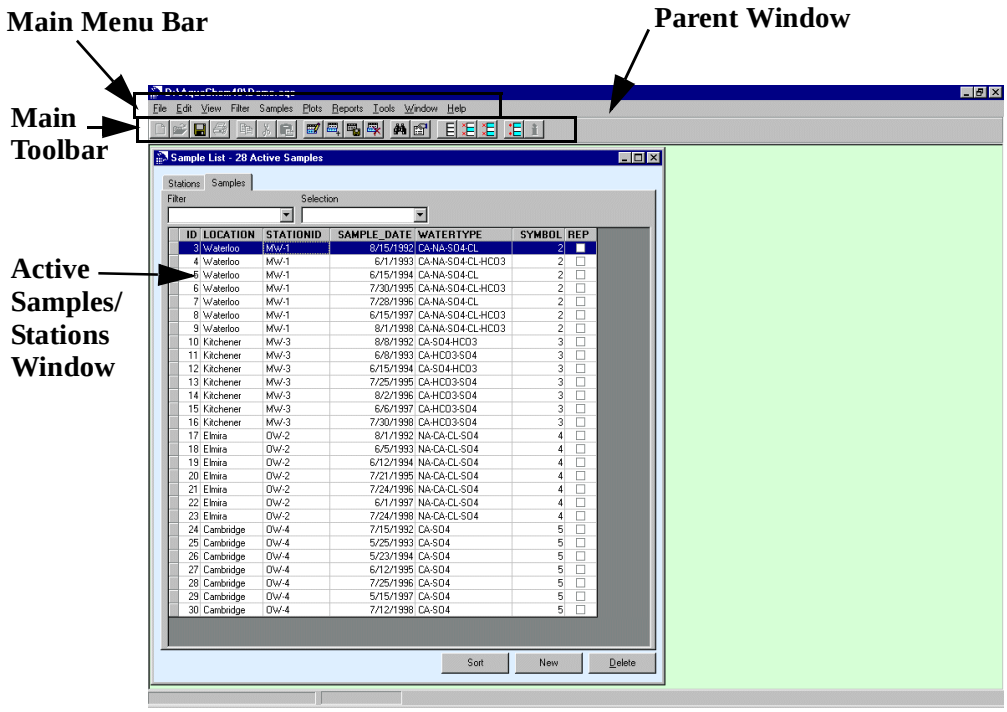
Once you have opened the v.3.7 project, you will see that a **StationID** has been assigned to each of your samples. AquaChem will create the StationID from a combination of the **Site** and **Location** fields from your v.3.7 project; these fields will be separated by a period. For example, your StationID will be **Site.Location** (ex. MW-1.Waterloo). In AquaChem v.4.0, the Site field has been replaced by a Station Name field.

NOTE: When opening a database from v.3.7, please ensure that each of the following files reside within the same project folder: Filename.HC3, Filename.CFG, and Filename.MSK

Data sets from AquaChem v 3.6 cannot be imported directly into v.4.0, due to different data structures and numeric date formats. In order to open a data set from v.3.6, first export your dataset out to a text file using the **File > Export ASCII** command in v.3.6. Then open AquaChem version 4.0, create a new database and use the **File > Import** command to load in this dataset.

1.5 AquaChem Interface Layout

After opening an AquaChem database file, a screen layout similar to the following figure will appear.



Parent Window is the main AquaChem window which houses all other windows.

Main Menu Bar contains specific menus for graphs and dataset. Depending upon the currently selected window, each window has a distinct set of menu options. A detailed description of each main menu options associated with various windows is provided in Chapter 3: AquaChem Menu Commands.

Main Toolbar contains specific tool buttons for different options. A detailed description of each main toolbar item is provided in section 1.6 of this chapter, AquaChem Toolbar.

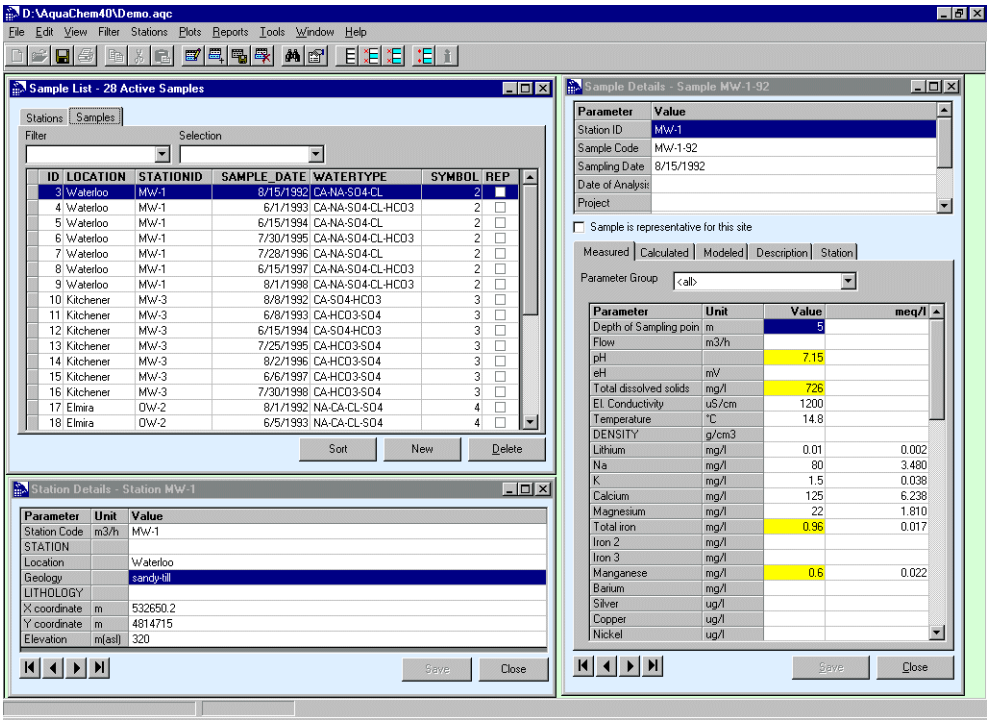
Active Samples/Stations Window will always appear when you open an AquaChem database and will remain on-screen as long as the project database is open (i.e. the Active Samples/Stations window cannot be closed unless the project database is closed). This window displays the list of samples and stations in the currently selected database. Two further windows can be accessed through the **Active Samples/Stations** tab to display and manipulate the dataset:

- **Sample Details Window** contains details for the selected sample.
- **Station Details Window** contains details for the selected station.

The following remaining ‘Child’ windows are used to display and manipulate the data which can be accessed through the main menu commands:

- **Table View** available under **View** menu allows you to view and edit the data in the database as a table.
- **Template Designer** available under the **File** menu contains options for designing print templates for plots and reports.
- **Reports** loads pre-defined data analysis reports, or user-designed reports. The **Report Designer** available under the **Reports** contains options for designing data reports.
- **Tools** loads several tools for data analysis and interpretation. **Modeling > PHREEQC** available under the **Tools** loads the interface for the PHREEQC modeling utility, and provides direct links to PHREEQC-I or PHREEQC for Windows.

AquaChem follows most standard Windows interface conventions. Each window can be minimized to the bottom of the Parent window and re-opened as needed. Likewise, window sizes can be adjusted by dragging and releasing the corners of the window frame. Windows can be arranged (as shown below for example) on the Parent window using the **Windows > Tile Horizontal** or **Tile Vertical** command which are available from all menus.



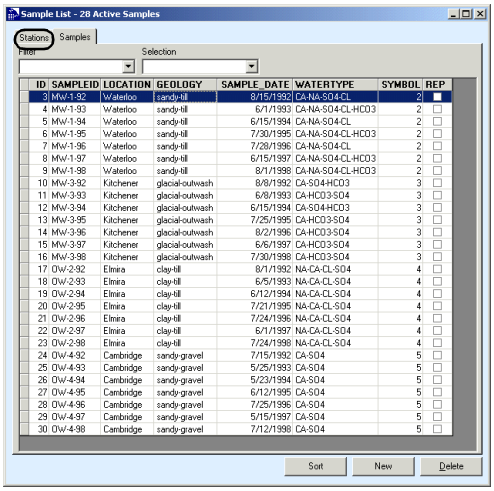
AquaChem Interface Layout

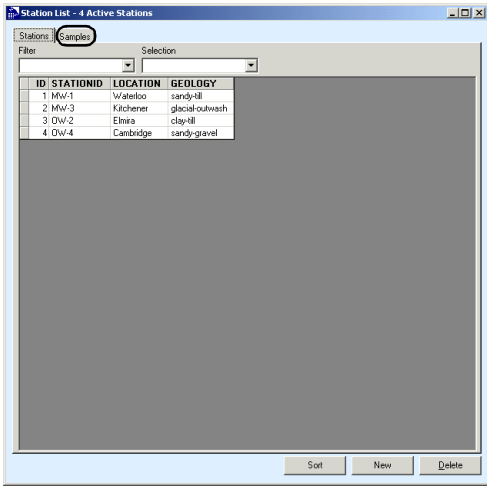
The following section summarizes the features of each of the main AquaChem windows.

Active Samples/Stations Window

As mentioned in the introduction, version 4.0 of AquaChem follows a database hierarchy of stations followed by samples. This means that each sample must have a corresponding station. When you create a new sample, a corresponding station with a unique identifier must be assigned to it.

The **Active Sample/Stations** window contains summarized information about every active sample and station in the database; the fields in this window are read-only which means that fields in this window cannot be edited. This window contains two tabs: **Stations** and **Samples**. Clicking on these tabs displays the following windows.





The first column in the these windows will always contain an ID value; each sample and station in your database will have a unique database ID value. This allows AquaChem to manage the data and perform internal calculations.

> **NOTE**: The internal database ID value cannot be edited, nor can this column be removed from the active list. This ID is automatically created when you create a new sample or station.

In addition to the ID column, there will be columns containing sample or station description parameters. These columns can be modified and the sorting options can be modified as well. For more details on sorting the active list, please see the **View > Options - Active List** section in Chapter 3.

The bottom of the **Active Sample/Stations** window contains the following three buttons:

The **[Sort]** button will load the sort options for the active list. This will allow you to change which parameters appear in the active list and their order.

The **[New]** button will create a new sample or station, depending on which mode is active (i.e. which tab is selected).

The **[Delete]** button will delete the selected sample or station.

In order to edit the data for a specific sample or station, you need to open the **Sample Details** or **Station Details** window. These windows are explained in greater detail in the following sections.

Sample Details Window

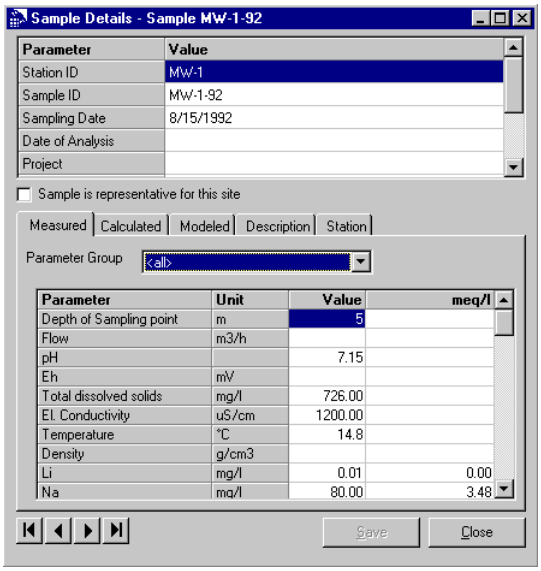
The **Sample Details** window is a read/write window, which means data can be entered, saved, and read from this window. Individual samples can be created, edited, or viewed using this window.

To load this window for one of the samples in your active list, you can:

- select a sample from the active list and **double-click** the left mouse button on it; OR
- select a sample from the active list and press the **<Enter>** key on your keyboard; OR
- select a sample from the active list and click **Sample > Edit** from the main menu; OR
- right-click the sample from the active list and select **[Edit]**.

An example of the **Sample Details** window is shown below:

To enter data in the **Sample Details** window, simply double-click in the desired field and type in the appropriate information. Alternatively, data can be imported into your database using the **Import** feature (see the **File > Import** section for more details).



The **Sample Details** window is separated into two frames: the top frame includes general details on the sample (Sample Description Parameters), and the bottom frame contains the **Measured**, **Calculated, Modeled**, **Description** and **Station** tabs.

Data can be entered for the Station Description parameters at the top of this window, and in the **Measured** and **Description** tabs in the bottom half of this window. Under the **Measured** Parameters tab, you will see the label **Parameter Group** with a corresponding combo box. This allows you to select different groups of Measured Parameters, and focus on just desired groups (for example you may want to view just Anions or Cations). The **Hide Non-Detects** group will hide all parameters for which there is no data recorded, and display only those samples which have measured values.

For Measured Parameters, you may also right-mouse click on a parameter in order to view the Parameter Details. The Parameter Details displays all the data available for the selected parameter including description, formula weight, and the CAS Registry number.

The **Calculated** tab contains function values based on measured data from the current sample. These entries cannot be edited (this data is read-only).

The data in the **Modeled** tab is obtained from PHREEQC simulations (as such, there will be no values for Modeled Parameters when you build a new database). There are three ways in which you can copy PHREEQC results into the **Modeled** tab:

1. You may click the PHREEQC button at the bottom of the window, and PHREEQC will calculate the Saturation Indices for the available Modeled Parameters. This will be done only for the selected sample;

2. You may select multiple samples in the Active Samples list, and use the menu option **Tools > Modeling > Calculate Sat. Indices and Activities**.

3. You may manually create a PHREEQC input file, using the **PHREEQC (Basic)** option under the **Tools > Modeling** menu. This option is recommended only for users that are familiar with the PHREEQC

modeling program. The results from the simulation must be manually inserted into your AquaChem samples.

The data under the **Station** tab is read-only, and as such cannot be edited. The Station tab contains information on the station which corresponds to the current sample. To edit the station parameters, open the **Station Details Window** as described in the next section.

The scroll buttons at the bottom of the **Sample Details Window** can be used to scroll through the Sample Details for other samples:

The order of these buttons (from left to right) is as follows:

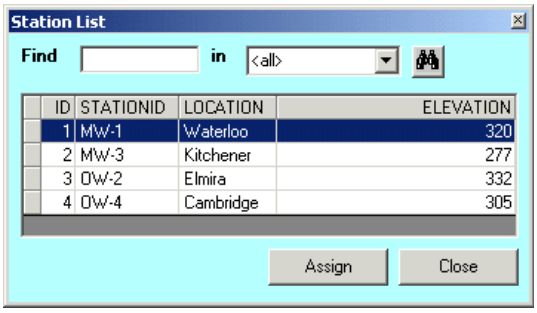
First sample - loads the sample details for the first sample in your active list.

Previous sample - loads the sample details for the previous sample in your active list.

Next sample - loads the sample details for the next sample in your active list.

Last sample - loads the sample details for the last sample in your active list.

The first field in the Sample Details window is the **Station ID**. As mentioned earlier, every sample must have a station assigned to it. To assign a station to a sample, click once in this field then click the ... button which will appear near the right side of this field. Alternatively, you may click **Samples > Assign Station** from the main menu. This will load a list of available stations, similar to the dialogue shown to the right side.



From this dialogue, you may select a station directly from the list; or if you have a long list of stations, the **Find** feature at the top of this window can be helpful. Simply enter a search query in the **Find** field, and choose a category from the combo box beside this field. Then press the **Find** icon to run a search for this term.

Once you have located the desired station for this sample, press the **[Assign]** button at the bottom of this dialogue and this will return you to the Sample Details window.

When you are finished in the Sample Details window, press the **[Save]** button at the bottom to save new data and/or changes to your database. Once you are finished, press **[Close]** to return to the Active List.

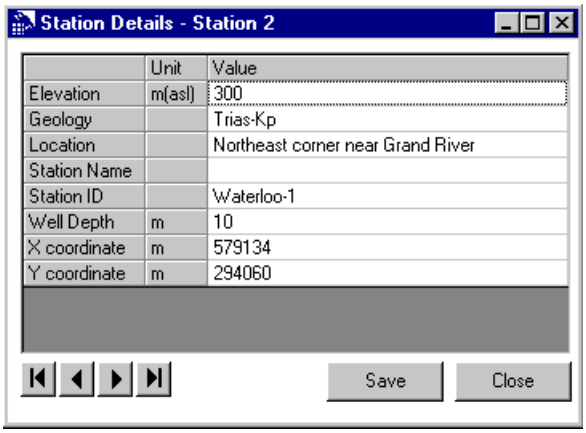
Station Details Window

The **Station Details** window is a read/write window, which means data can be entered, saved, and read from this window. Individual stations can be created, edited, or viewed using this window.

To load this window for one of the stations in your active list, you can:

- select the station from the active list, then **double-click** the left mouse button on it; OR
- select the station from the active list, then press the **<Enter>** key on your keyboard; OR
- select the station from the active list and click **Station > Edit** from the main menu; OR
- right-click on the station from the active list and select **[Edit]**.

An example of the **Station Details** window is shown below.



To enter data in the **Station Details** window, simply double-click in the desired field and type in the appropriate information. Alternatively, data can be imported into your database using the Import feature (see the **File > Import** section for more details). To save new data and/or changes to the database for this station, press the **[Save]** button at the bottom of this window. Once you are finished, press **[Close]** to return to the active list.

The scroll buttons at the bottom of this window are similar to the Sample Details window; these buttons can be used to scroll through the details for other stations in your active list.

Plots Window

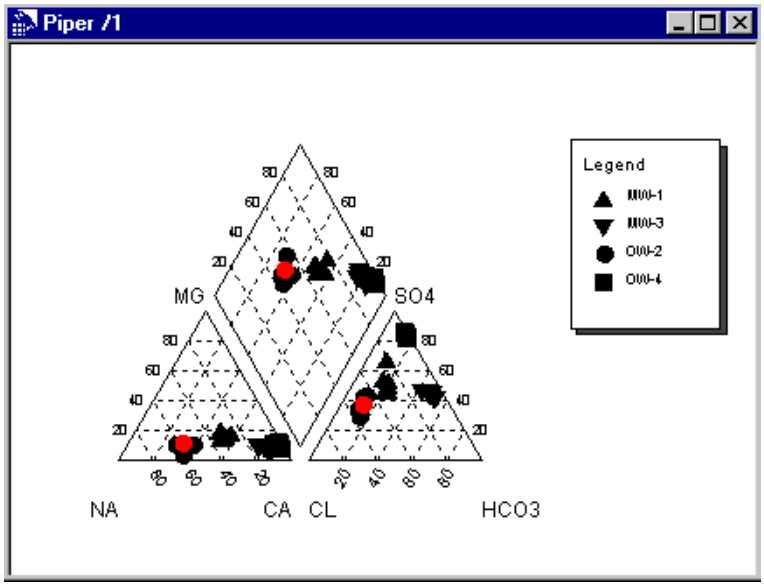
AquaChem provides a comprehensive selection of 19 different plotting techniques commonly used for aqueous geochemical data analysis and interpretation. Each of these plot types can be used to graphically represent information for all samples in the Active Samples List, or for selected samples only.

To create a new plot:

- Ensure the Active List is the current active window.
- Select **Plots > New** from the main menu.
- Choose the desired plot type from the list in this menu.
- Modify the plot options or click **[OK]** to accept the defaults.

This will create a Plot window displaying the selected plot for all samples in the Active Samples List.

An example below shows a plot window containing a **Piper** plot:



Any samples selected in the Active List will be highlighted on the Piper plot in red. These sample points can be labelled, and the shapes and sizes of the symbols can also be modified. Likewise, the plot options can be adjusted to show just the selected samples, or all the current active samples available in your database.

It is important to remember that the data plotted on all open plots are directly linked to the database samples. Any changes to the data are immediately reflected in each of the open graphs. Clicking a data point on the graph will highlight the corresponding sample in the Active samples list window (the corresponding data point in all other open plot

windows will also be highlighted). This can be effective for identifying outlier points on the plot. Similarly, selecting a sample in the active list will highlight the corresponding data point on all open graphs (in red). Changing the number of samples in the active list automatically updates ALL open plots.

For more details on the various Plots and their respective options, please refer to Chapter 4: **Plots**.

Table View

The **Table View** window is loaded when you select **View > Table View** from the main menu. You can then load the **Default** table view, or use the **Create** option to design your own Table (spreadsheet) View.

For more details on the Table View options, please see the **View > Table View** section in Chapter 3.

Reports Window

A **Report** window provides reported and/or calculated information for a selected sample, group of samples, or all active samples in the database. The reports can be produced by selecting a sample from the active list and then selecting one of the report types from the **Reports Menu** option.

The text reports can be edited, printed, or saved to a TXT or CSV file. AquaChem generates several types of reports. Using the **Report Designer**, you can create and customize your own reports, to display whatever data and/or calculations you desire.

For more details, please refer to Chapter 5: **Reports**.

Tools

AquaChem provides you with the following pre-defined data analysis tools:

- AquaChem Function
- Decay Calculator
- Find Missing Major Ion
- Formula Weight Calculator
- Volume Concentration Converter
- Special Conversions
- Species Converter
- Unit Conversions

In addition, there are also **Look Up Tables** available under the **Tools Menu**, and options for the linking to the PHREEQC interface.

For more details, please refer to Chapter 6: **Tools**

PHREEQC Interface

AquaChem includes a direct link to the PHREEQC modeling program, version 2.8. The GUI has been redesigned, and there is now an option to automatically save the PHREEQC simulation results back to your AquaChem database. You may also run the full version of PHREEQC-I or PHREEQC for Windows, utilizing more advanced options which are not available through the AquaChem interface.

For more details on PHREEQC and modelling, please refer to **Chapter 7**.

1.6 AquaChem Toolbar

This section describes each of the items in the AquaChem toolbar. Most toolbar buttons are context sensitive and react according to the active AquaChem window or dialogue. If there are no options available for the selected window or dialogue, the toolbar icons may become grey and inactive. The AquaChem toolbar is shown below.

For a short description of each item in the toolbar, place your mouse pointer over an icon and a hint will pop-up. The function of each toolbar item is described below:

New button creates a new database (only available if no other database is open)

Open button opens a database (only available if no other database is open)

Save button saves the current database file

Print button prints a plot, table, or a report

Copy button copies currently selected data, or copies a plot to the Windows Clipboard

Cut button cuts currently selected data

Paste button pastes currently copied (or cut) data

Edit button edits selected sample/station

Create button creates new sample/station

Export button exports data to a text file

Delete button deletes selected sample/station

Find button finds samples/stations

Options button views the options for sample/station list or Table View options

Show all button shows all samples/stations in the active list

Show only selected button shows only selected samples/stations in the active list

Omit selected button removes selected sample/station from the active list

Assign Symbol button assigns a symbol to the selected sample(s)

Identify button identifies sample data used on the selected plot(s)

2

Getting Started

This chapter is designed to serve as a ‘quick-start’ reference guide for those interested in getting started quickly using the most common features of AquaChem. You will follow a sample set of instructions, using the same data set that was used for the Demo database.

To begin, this chapter has been divided into sections for your convenience - feel free to read through the entire chapter, or jump directly to a section of interest.

Creating a New Database

- Importing Data
- Assigning Symbols

Creating Plots

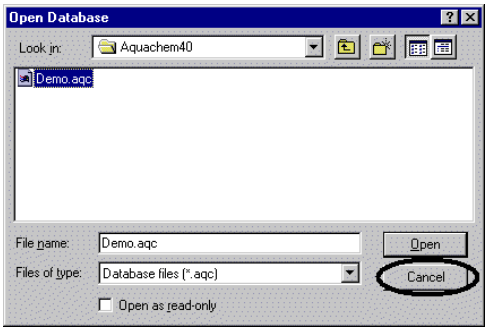
- Plot Options
- Printing Plots
- Saving Plots as Graphics File

Creating Reports

- Reports Options
- Saving Reports
- Printing Reports

2.1 Creating a New Database

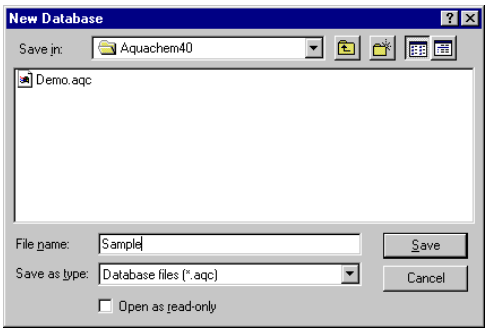
When you first load AquaChem, an **Open Database** dialogue will appear. You have the option of loading the Demo.AQC project, or to create a new project. To create a new project, press **[Cancel]** when this dialogue appears.



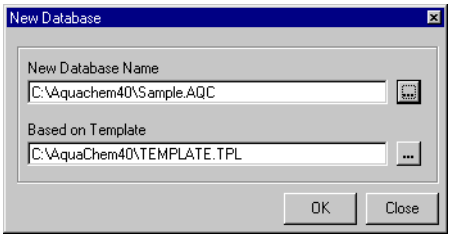
After pressing **[Cancel]**, you will see a blank AquaChem window indicating there is no database loaded.

To create a new database:

- Select **File** from the main menu and then select **New**. A **New Database** dialogue will appear as shown below.



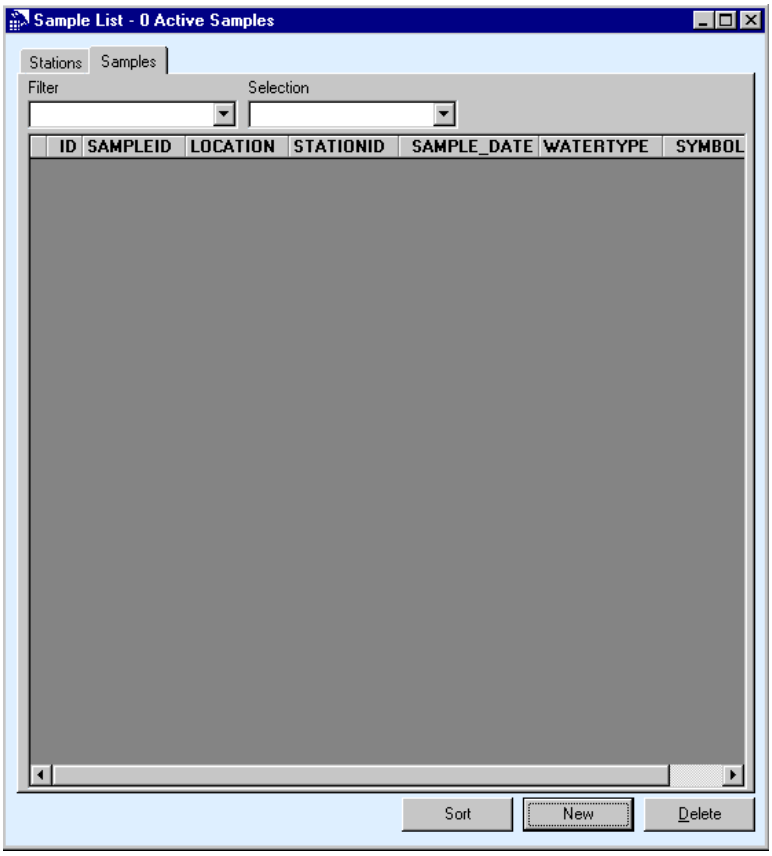
- Browse to the appropriate folder (the default folder will be your AquaChem40 installation folder, *C:\AquaChem40*).
- Type in the name of the new database, and click **[Save]**. (For this demonstration, the file will be called **Sample.aqc**).
- You will then see the following **New Database** confirmation dialogue.



- Below the **New Database Name** field, in the **Based on Template** field, you must specify a database template file to use for the creation of your database. If you are a new user to AquaChem, it is recommended that you use the **Template.TPL** file as the starting template for your database (the default). After becoming more experienced with the program, you can create new templates and use these for future databases.
- Click **[OK]** once you are finished entering the database (.AQC) and template (.TPL) name.

NOTE: It is recommended that database filenames contain a combination of letters and numbers only. The filename and directory path should NOT contain spaces, accents, or other characters.

AquaChem will then automatically create a blank database file using the associated database template file containing the data structure for each record in the database. A blank database is shown below:



At this point, you can now begin to enter your sample data into the database. You have two options for data entry:

- Data can be entered manually; or
- Data can be imported from a text file.

The most convenient option for large data sets is to import the data from a text file; this will be demonstrated below. If you enter your data manually, be sure to first create a minimum of one station, so that you have a pre-existing station to assign to your samples. If the data is imported, the station data can be imported the same time as the sample date.

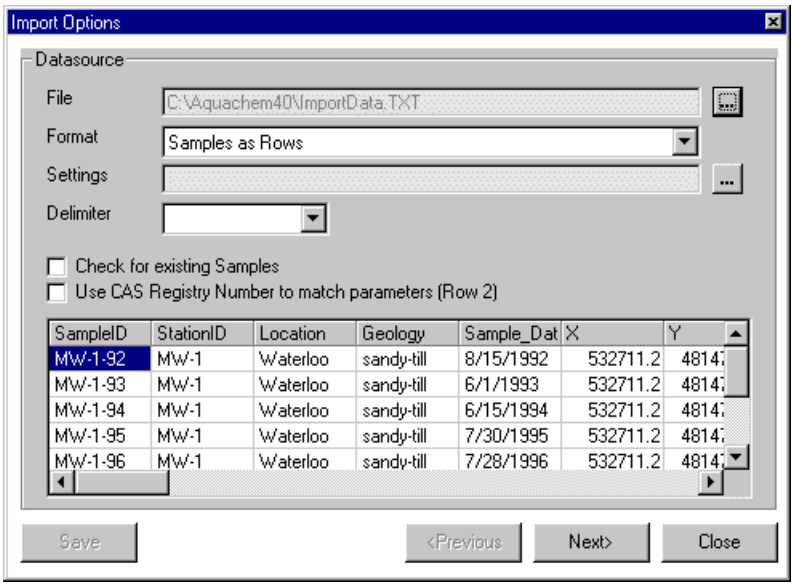
Before proceeding with the import option, you should ensure that your source file containing your water analysis data is properly formatted. For your convenience, an Excel template is provided with AquaChem, which includes some of the most common **Sample** and **Station** parameters. This file is called **Import_Template.XLS** and can be found in the root AquaChem installation folder. If you wish, you may use this file for your data set. Simply enter your data, then **Save** the Excel file as "Tab-Delimited Text", and proceed with the import options.

2.1.1 Importing Data

To import sample data into your AquaChem database, please follow these steps:

- ☞ **File** from the main menu and then select **Import**
- ☞ ... button beside the **File** field to locate the source file
- ☞ **ImportData.txt** (located in the *C:\AquaChem40* directory). If necessary, browse to your AquaChem installation folder to locate this file.
- ☞ **[Open]**
- ☞ to select the import **Format** for the source file; **Samples as Rows** or **Samples as Columns**. For this demonstration, the **Samples as Rows** mode will be used.
- ☞ in the **Delimiter** field and select **Tab** from the combo box.

You should now see the ImportData.Txt file name in the **File** field, and a preview of file in the lower half of the dialogue (as shown below):



The remaining import options can be left as is.

☞ **[Next>]**

In the next dialogue, AquaChem requires you to match the fields in your text file to the required AquaChem parameter fields. For the **ImportData.txt** file, the column headings have already been prepared such that they precisely match up with the required AquaChem field headings. Therefore, there is no need to do manual matching. However, if there are blank fields in the AquaChem column, then this indicates that the parameter names in the text file are not identical to the Aquachem parameter names, and the fields could not be identified. For example, if your text file contained the parameter name '**Conductivity**', you must match this up to the AquaChem parameter Internal Key '**COND**'.

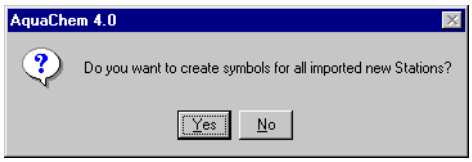
If necessary, please refer to Chapter 3: **File > Import**, for more details on matching parameters during the import.

☞ **[Next>]**

The next dialogue contains a list of the AquaChem parameters which were not matched up to parameters in the source file. This dialogue allows you to enter constant values for these parameters (optional). For example, if all of the imported samples belong to the same project or the same location you may fill the respective fields automatically during this step of the import. To skip this step, leave these fields blank.

☞ **[Next>]**

You will then see the following warning prompt:



This option allows you to automatically create one symbol for each unique station in the imported source file. These symbols will be created in the Station symbol group. This is a very help feature, which can aid in plotting your sample data later on.

☞ **[Yes]** to accept this feature.

The last dialogue in the import options, contains a summary of the import routine. Please check that all of your samples, stations, and parameters have been successfully imported.

☞ **[Close]**

Upon closing the import dialogue, you have the option of saving the Import Settings. To ignore this option,

☞ **[No]**

After successfully importing the data, you will return to the main database window showing your active **Samples** and **Stations**. For this data set, there should be 4 stations, with 7 samples taken from each station location, for a total of 28 samples.

2.1.2 Assigning Symbols

The next step to building a new AquaChem project is to assign symbols to your samples.

By default, a new database will include two symbol groups: a **Default** symbol group with just one symbol assigned to each sample, and a **Station** symbol group, with a unique symbol for each unique station in the database; the station symbols are automatically assigned to the appropriate corresponding samples. You may create new symbol groups, or add symbols to one of the existing symbol groups.

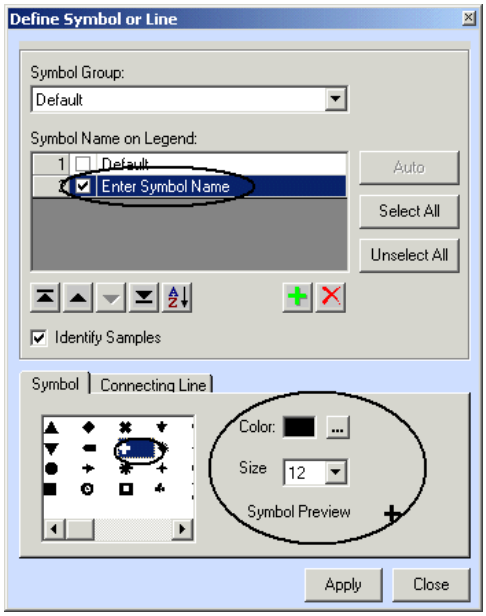
For this demonstration, you will add symbols to the **Default** group.

Follow the instructions below to create new symbols:

☞ **Plots** from the main menu and then select **Define Symbol or Line**

☞  below the **Symbol Group**, and ensure the **Default** symbol group is selected.

☞  button and a new field will be added to the list of symbols



type: **Waterloo** in the new line that is added

☞ **<Enter>** (on your keyboard) to accept the new name

You will now add three more symbols:

☞  button

type: **Kitchener** (for the new symbol)

☞ **<Enter>** on your keyboard

☞  button

type: **Elmira** (for the new symbol)

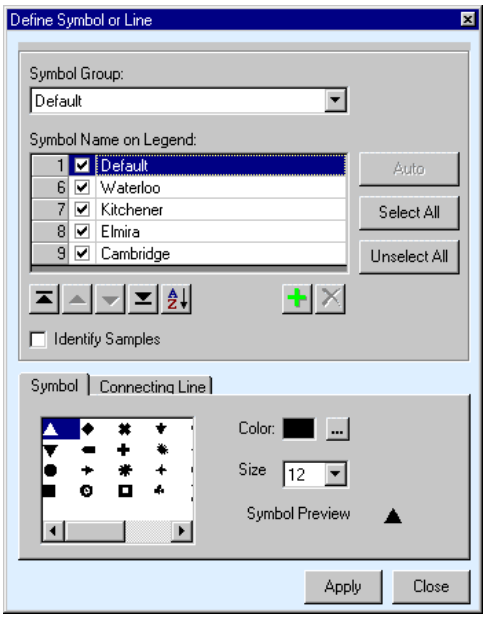
☞ **<Enter>**

☞ button

type: **Cambridge** (for the new symbol)

☞ **<Enter>**

Once you are finished, you should have five symbols listed for the **Default** symbol group, as seen in the figure below.



Next you need to define the necessary symbol properties:

☞ **Symbol #6 (Waterloo)** from the list

☞ Choose a symbol character from the list of available symbols (in the lower half of the dialogue). Simply click on the desired new symbol shape

☞ Choose a **Color** for the new symbol. To access the color options press the ... button beside **Color**, and select a color from the list of available colors

☞ Choose a **Size** for the symbol; the font sizes are available from the combo box beside **Size**. (Recommended size is 12pt.)

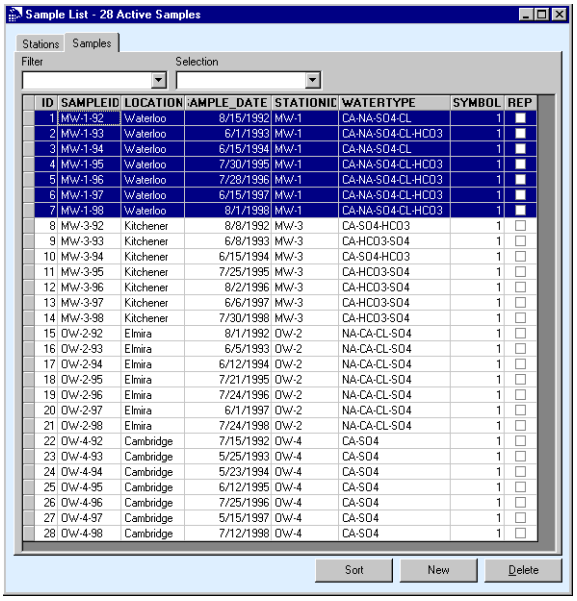
☞ **[Apply]** button, once you are finished.

Repeat these steps for the three other new symbols that were created.

Once you are finished creating the symbols and defining the symbol properties,

- ☞ **[Apply]**
- ☞ **[Close]**

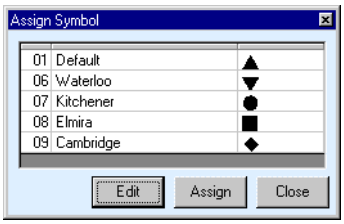
In your active samples list, you are ready to assign these symbols to the samples.



ID	SAMPLEID	LOCATION	AMPLE_DATE	STATIONID	WATERTYPE	SYMBOL	REP
1	MW-1-92	Waterloo	8/15/1992	MW-1	CA-NA-SO4-CL	1	
2	MW-1-93	Waterloo	6/1/1993	MW-1	CA-NA-SO4-CL-HCO3	1	
3	MW-1-94	Waterloo	6/15/1994	MW-1	CA-NA-SO4-CL	1	
4	MW-1-95	Waterloo	7/30/1995	MW-1	CA-NA-SO4-CL-HCO3	1	
5	MW-1-96	Waterloo	7/28/1996	MW-1	CA-NA-SO4-CL-HCO3	1	
6	MW-1-97	Waterloo	6/15/1997	MW-1	CA-NA-SO4-CL-HCO3	1	
7	MW-1-98	Waterloo	8/1/1998	MW-1	CA-NA-SO4-CL-HCO3	1	
8	MW-3-92	Kitchener	8/8/1992	MW-3	CA-SO4-HCO3	1	
9	MW-3-93	Kitchener	6/8/1993	MW-3	CA-HCO3-SO4	1	
10	MW-3-94	Kitchener	6/15/1994	MW-3	CA-SO4-HCO3	1	
11	MW-3-95	Kitchener	7/25/1995	MW-3	CA-HCO3-SO4	1	
12	MW-3-96	Kitchener	8/2/1996	MW-3	CA-HCO3-SO4	1	
13	MW-3-97	Kitchener	6/6/1997	MW-3	CA-HCO3-SO4	1	
14	MW-3-98	Kitchener	7/30/1998	MW-3	CA-HCO3-SO4	1	
15	OW-2-92	Elmira	8/1/1992	OW-2	NA-CA-CL-SO4	1	
16	OW-2-93	Elmira	6/5/1993	OW-2	NA-CA-CL-SO4	1	
17	OW-2-94	Elmira	6/12/1994	OW-2	NA-CA-CL-SO4	1	
18	OW-2-95	Elmira	7/21/1995	OW-2	NA-CA-CL-SO4	1	
19	OW-2-96	Elmira	7/24/1996	OW-2	NA-CA-CL-SO4	1	
20	OW-2-97	Elmira	6/1/1997	OW-2	NA-CA-CL-SO4	1	
21	OW-2-98	Elmira	7/24/1998	OW-2	NA-CA-CL-SO4	1	
22	OW-4-92	Cambridge	7/15/1992	OW-4	CA-SO4	1	
23	OW-4-93	Cambridge	5/25/1993	OW-4	CA-SO4	1	
24	OW-4-94	Cambridge	5/23/1994	OW-4	CA-SO4	1	
25	OW-4-95	Cambridge	6/12/1995	OW-4	CA-SO4	1	
26	OW-4-96	Cambridge	7/25/1996	OW-4	CA-SO4	1	
27	OW-4-97	Cambridge	5/15/1997	OW-4	CA-SO4	1	
28	OW-4-98	Cambridge	7/12/1998	OW-4	CA-SO4	1	

- ☞ Select the first seven samples in your sample list. To do so, click on the first sample, hold down your left mouse button, and drag your mouse down to the 7th sample.
- ☞ **Samples** from the main menu and then select **Assign Symbol** from the main menu (or use the Assign Symbol icon in the tool bar).

The **Assign Symbol** dialogue will list the available Symbol group names and the corresponding symbol, as defined earlier.



- ☞ Symbol **06 Waterloo**
- ☞ **[Assign]**

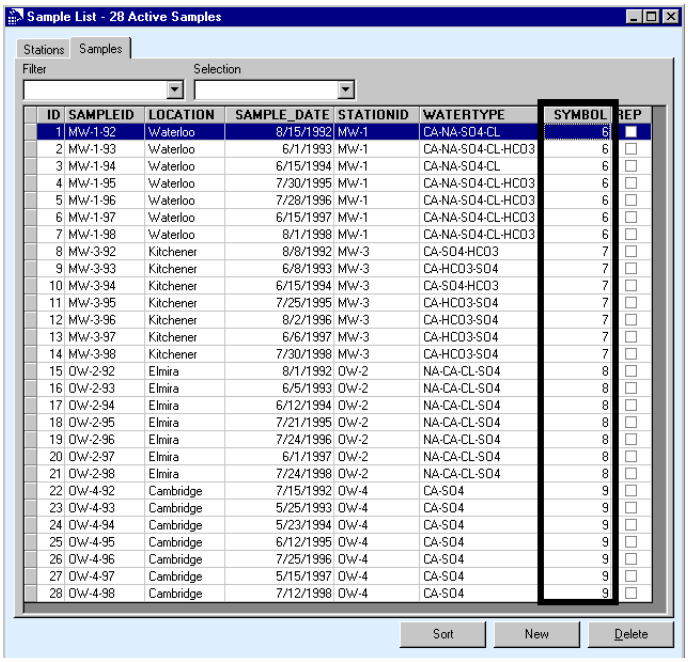
- **[Close]**

You will now assign symbols to the next group of samples.

- Select the samples from the **MW-3** Station (Kitchener) (Samples 8 to 14)
- **Samples** and then select **Assign Symbol**
- Symbol **07 Kitchener**
- **[Assign]**
- **[Close]**

Repeat these steps to assign symbols to the remaining samples for stations OW-2 and OW-4.

Once you are finished, each of your samples should have a corresponding symbol which relates to the location of that sample. In the active list of samples, there is a column heading **Symbol** which indicates the Symbol group that is assigned to each sample. You should see Symbols 6, 7, 8, and 9 in your sample list, as shown below.



ID	SAMPLEID	LOCATION	SAMPLE_DATE	STATIONID	WATERTYPE	SYMBOL	REP
1	MW-1-92	Waterloo	8/15/1992	MW-1	CA-NA-SO4-CL	6	
2	MW-1-93	Waterloo	6/1/1993	MW-1	CA-NA-SO4-CL-HCO3	6	
3	MW-1-94	Waterloo	6/15/1994	MW-1	CA-NA-SO4-CL	6	
4	MW-1-95	Waterloo	7/30/1995	MW-1	CA-NA-SO4-CL-HCO3	6	
5	MW-1-96	Waterloo	7/28/1996	MW-1	CA-NA-SO4-CL-HCO3	6	
6	MW-1-97	Waterloo	6/15/1997	MW-1	CA-NA-SO4-CL-HCO3	6	
7	MW-1-98	Waterloo	8/1/1998	MW-1	CA-NA-SO4-CL-HCO3	6	
8	MW-3-92	Kitchener	8/8/1992	MW-3	CA-SO4-HCO3	7	
9	MW-3-93	Kitchener	6/8/1993	MW-3	CA-HCO3-SO4	7	
10	MW-3-94	Kitchener	6/15/1994	MW-3	CA-SO4-HCO3	7	
11	MW-3-95	Kitchener	7/25/1995	MW-3	CA-HCO3-SO4	7	
12	MW-3-96	Kitchener	8/2/1996	MW-3	CA-HCO3-SO4	7	
13	MW-3-97	Kitchener	6/6/1997	MW-3	CA-HCO3-SO4	7	
14	MW-3-98	Kitchener	7/30/1998	MW-3	CA-HCO3-SO4	7	
15	OW-2-92	Elmira	8/1/1992	OW-2	NA-CA-CL-SO4	8	
16	OW-2-93	Elmira	6/5/1993	OW-2	NA-CA-CL-SO4	8	
17	OW-2-94	Elmira	6/12/1994	OW-2	NA-CA-CL-SO4	8	
18	OW-2-95	Elmira	7/21/1995	OW-2	NA-CA-CL-SO4	8	
19	OW-2-96	Elmira	7/24/1996	OW-2	NA-CA-CL-SO4	8	
20	OW-2-97	Elmira	6/1/1997	OW-2	NA-CA-CL-SO4	8	
21	OW-2-98	Elmira	7/24/1998	OW-2	NA-CA-CL-SO4	8	
22	OW-4-92	Cambridge	7/15/1992	OW-4	CA-SO4	9	
23	OW-4-93	Cambridge	5/25/1993	OW-4	CA-SO4	9	
24	OW-4-94	Cambridge	5/23/1994	OW-4	CA-SO4	9	
25	OW-4-95	Cambridge	6/12/1995	OW-4	CA-SO4	9	
26	OW-4-96	Cambridge	7/25/1996	OW-4	CA-SO4	9	
27	OW-4-97	Cambridge	5/15/1997	OW-4	CA-SO4	9	
28	OW-4-98	Cambridge	7/12/1998	OW-4	CA-SO4	9	

The samples are now ready to be plotted.

2.2 Creating Plots

AquaChem allows you to plot your sample data using 19 different plot types. For this exercise, you will create a simple Piper plot which distinctly show the four different sample groups. For more details on the AquaChem plots and the plot options, please refer to Chapter 4.

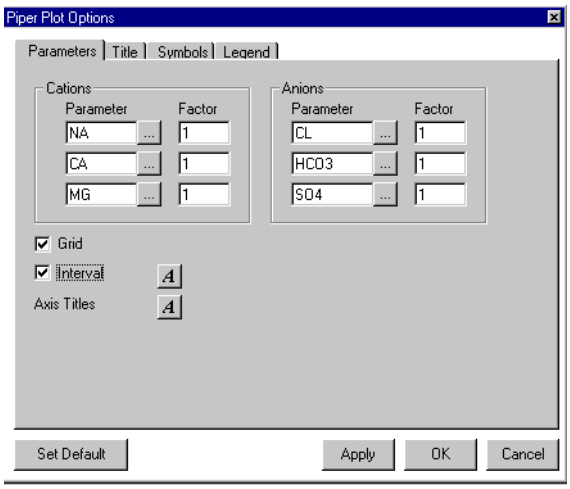
☞ **Plots** from the main menu, then select **New** and then **Piper**

A **Piper Plot Options** dialogue will appear with default plot settings. The following section describes some of the generic plot options.

To create the plot using the default plot options, press **[OK]** and proceed to the next section titled **Printing Plots**.

2.2.1 Plot Options

There are many common graphical features and options for each plot. When you select any of the graph types to plot (for example Piper plot), a plot options dialogue will appear with default settings for all of the necessary parameters and settings. For most plot types, the **Plot Options** dialogue contains four tabs: **Parameters**, **Title**, **Symbols**, and **Legend**.



Parameters Tab

Contains information on the parameters/series used in the plot, **Axis Labels** and font options, **Axis Titles** and **Intervals**, and toggles to turn the plot gridlines or axis intervals on/off.

Title Tab

Contains options for **Plot Title** font size, **Position**, and **Alignment**.

Symbols Tab

Contains options for symbols used in the plot, **Symbol Labels**, **Scaled Symbol Size** options, etc.

Legend Tab

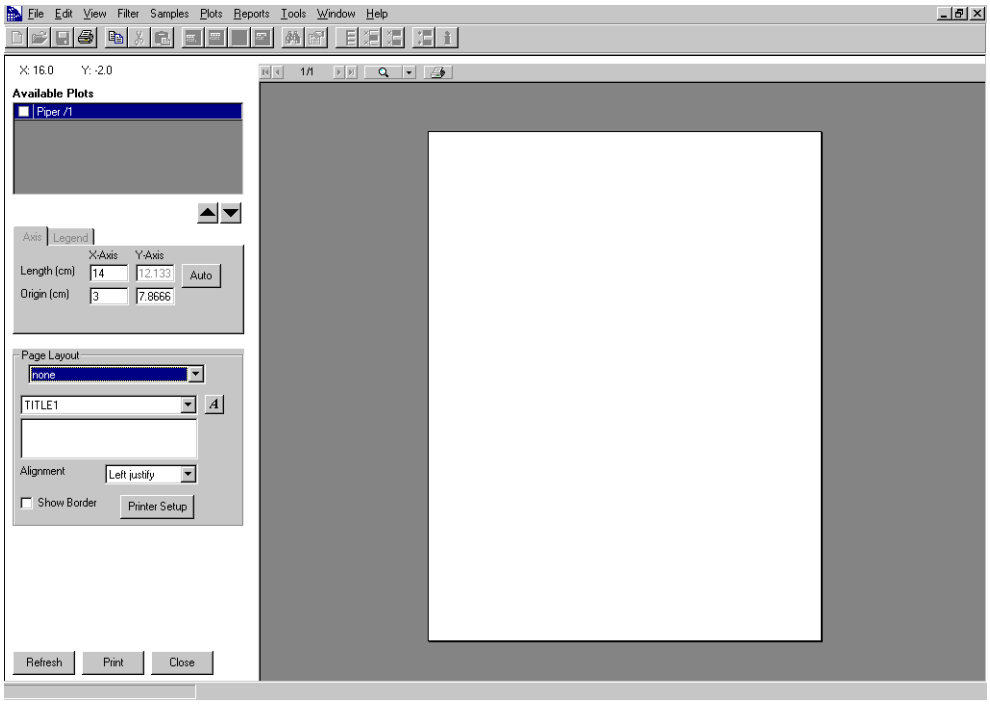
Contains options for displaying a **Plot Legend**, Legend **Title**, and display features.

2.2.2 Printing Plots

Once you have prepared the desired plot(s), you are ready to print.

☞ **File** from the main menu and select **Print,** or press the Print icon in the tool bar.

You should then see a **Print Options** window, as seen below.



The Print Options allow you to choose which plots will be printed, their position, size, and which plot template will be used, and other Windows page setup options.

A list of **Available Plots** will appear in the upper-left corner of this window. This list represents the plots which are currently open in AquaChem and are available for printing.

Select the plots you want to print by placing a check mark in the box beside the appropriate plot name.

To select the Piper plot for printing,

- ☞ Click once in the box beside **Piper /1**, and a check mark will be added to the box. This plot should now appear in the preview window (on the right).

To load additional plots, simply click once with your mouse in the box beside the plot name.

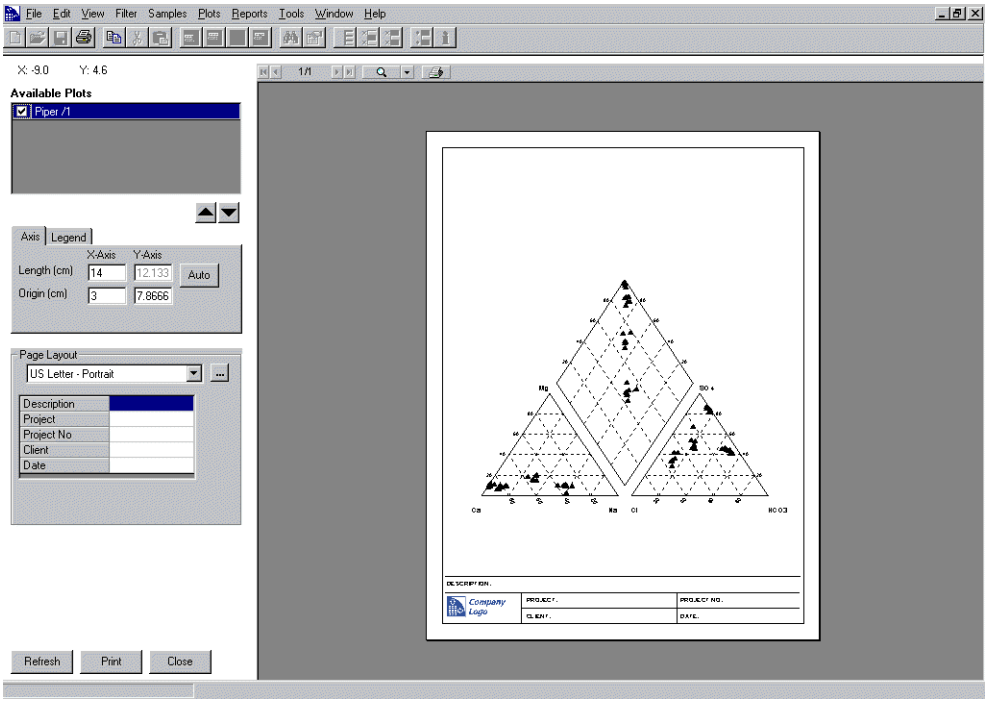
The plot will be automatically sized to fit the page layout. If the default page settings are not suitable, you can manually change the position of each plot using the options provided in the **Axis** tab (**Length** and **Origin**).

Next, you can select the page layout by choosing a print template. The print template will allow you to enter information on the page footer such as project information, sample information, and company information.

Under the **Page Layout** options (on the left side of the window), you will see the default template setting is **none**. For this exercise, you will load one of the AquaChem printing templates.

- ☞  from the combo box and select the **US-Letter Portrait** template

A list of plot descriptors will appear in the **Page Layout** dialogue, and the print preview window will be automatically updated to reflect the selected template settings. Your Print options window should now be similar to the one seen below:



Next, you will fill in the project specific plot description fields under the **Page Layout** options. Press the **<Enter>** key after each entry:

DESCRIPTION:

type: Piper plot of samples collected from 1992 to 1998

PROJECT:

type: Demo Project

PROJ #:

type: 2003-1

CLIENT:

type: Your name or a client's name.

DATE:

type: Current date

NOTE: The Waterloo Hydrogeologic logo shown in the bottom of the page can be easily replaced with your own company logo. This can be done using the **Template Designer** option. This option is not explored in this exercise.

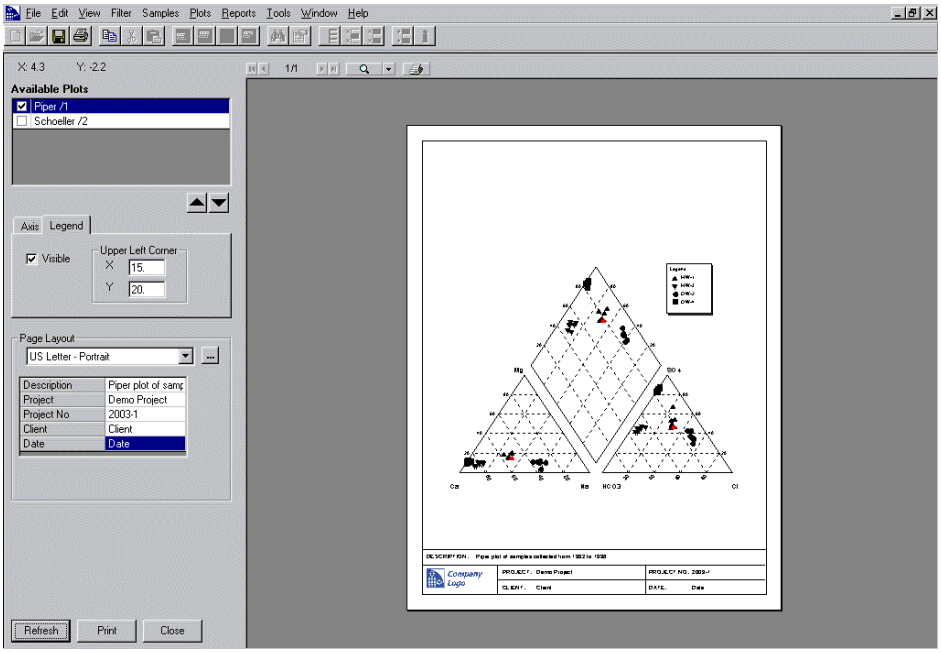
Next, if you have added a legend for your plot, you must add this legend to the printed page, and position it on the page.

- ☞ **Legend** tab (below the list of **Available Plots**, and beside the **Axis** tab).
- ☞ **Visible** (click once in this box) to activate the legend for the Piper Plot.

The **Piper** plot legend will appear in the upper-left corner of the page. To move the legend,

- ☞ **X-Axis** field and enter a value of 15.
- ☞ **Y-Axis** field and enter a value of 20.
- ☞ **[Refresh]** button (in the lower left corner) to refresh the Print Preview.

If you have loaded the plot successfully, your display should be similar to the one shown below:



- ☞ **[Print]** button (in the lower left corner) to print the plot to a printer.
- ☞ **[Close]** to close the print options window and return to the AquaChem active samples list.

2.2.3 Saving Plots as Graphics File

Upon returning to the main AquaChem window, you will see that the active sample list window is open, and you should still have the Piper Plot window open. In addition to printing the Piper plot, you will now save this plot as a graphics file so that it may be inserted into an external report.

- **Piper plot window** to make this the active window
- **File** from the main menu, and then choose **Save,** or press the **Save** icon in the Toolbar.

You will then be prompted to enter a filename for the plot. Browse to the desired folder on your computer, then enter a name for the file. For this demonstration, you will save the file in the AquaChem folder.

type: **Piper** as the filename for the plot

- **[Save]**

The plot will be saved as a .WMF (Windows MetaFile) graphics file. This file can be opened using most conventional graphics editors, or the file can be directly inserted into a word processor application.

-  button in the upper-right corner of the **Piper Plot window**, to close this plot window.

In the next section, the Report options will be briefly demonstrated.

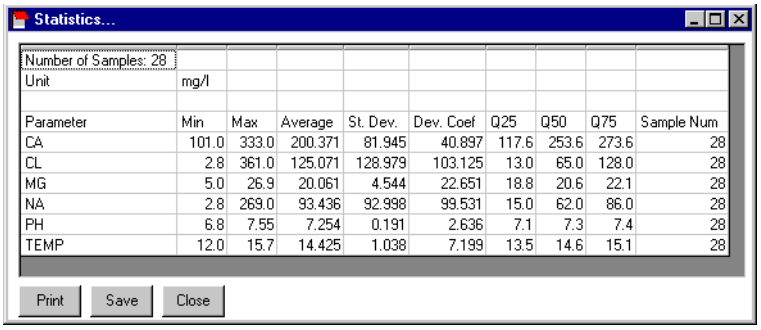
2.3 Creating Reports

AquaChem allows you to choose from 7 data analysis reports, and also allows you to customize your own reports. For this demonstration, you will briefly examine the generic Report options and create a Statistics Report. The **Statistics Report** provides a statistical summary of selected parameters for all active samples in your database. For more details on Reports, please refer to Chapter 5.

To create a **Statistics Report** for all samples in the active list:

- **Reports** from the main menu and then choose **Statistics**
- **[OK]** (to accept the default report settings)

The **Statistics** report window should be shown on your display, similar to the one below.



Parameter	Min	Max	Average	St. Dev.	Dev. Coef	Q25	Q50	Q75	Sample Num
CA	101.0	333.0	200.371	81.945	40.897	117.6	253.6	273.6	28
CL	2.8	361.0	125.071	128.979	103.125	13.0	65.0	128.0	28
MG	5.0	26.9	20.061	4.544	22.651	18.8	20.6	22.1	28
NA	2.8	269.0	93.436	92.998	99.531	15.0	62.0	86.0	28
PH	6.8	7.55	7.254	0.191	2.636	7.1	7.3	7.4	28
TEMP	12.0	15.7	14.425	1.038	7.199	13.5	14.6	15.1	28

The minimum, maximum, arithmetic mean, standard deviation, as well as other values of interest will be calculated for the selected database parameters.

NOTE: You may need to adjust the column widths in order to see the full column headings and the entire contents of the report.

The following section describes some of the options available for Reports.

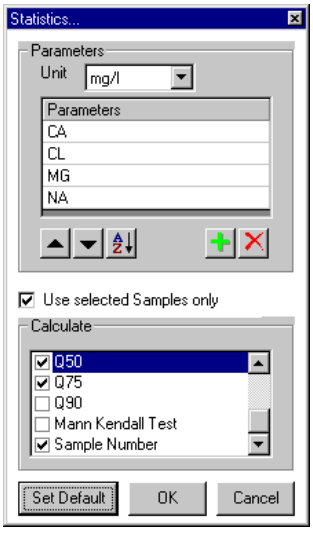
2.3.1 Reports Options

To see statistical analysis for other parameters, you need to return to the Report options.

To do so, click **View** from the main menu and then choose **Options**.

The **Statistics...** report options dialogue (on the right side) allows you to add or remove parameters from report list, and to specify which statistical analysis will be calculated.

To add a new parameter,



- ☞ button
- ☞ Select the desired parameter from the dialogue that appears.
- ☞ **[Select]**
- ☞ **[Close]**

To remove a parameter from the list,

- ☞ Select the parameter to be removed
- ☞ button

To add a new analysis to the Statistics Report, simply place a check mark in the box beside the desired statistical analysis.

- ☞ **[OK]** to re-create the report with these new options.

Once you are finished, you can save or print the report.

2.3.2 Saving Reports

Reports can be printed or saved to multiple file formats. The supported file formats are .TXT and CSV.

NOTE: The pre-defined reports in AquaChem can be saved as .TXT and CSV. The user-defined reports (e.g. Sample Summary Report created using the Report Designer) can be saved as .HTM or .RTF format.

To save the report,

- ☞ **[Save]** button at the bottom of the report window

type: a filename for the report

- ☞ Select the file type
- ☞ **[Save]**

2.3.3 Printing Reports

To print any of the reports,

- ☞ **[Print]** button at the bottom of the Report window; or
- ☞ **File** from the main menu and then select **Print**, while the report window is active.

The Report will then be sent to your default Windows printer, or you may select another printer.

- ☞ **[Close]** located at the bottom of the Reports window, to close the window and return to the main AquaChem window.

This concludes the Getting Started chapter.

3

AquaChem Menu Commands

This chapter describes each of the items on the AquaChem menu bar. Similar to the AquaChem Toolbar, the menu is context sensitive and main menu items are available only when the active list window is the currently selected window. In addition, menu items will become grey and inactive if there are no options available for the current mode.

In this chapter, you will find information on:

- File Menu
- Edit Menu
- View Menu
- Filter Menu
- Stations/Samples Menu
- Plots Menu
- Reports Menu
- Tools Menu
- Window Menu
- Help Menu

Following the menu items, you will find a section on the AquaChem database, which covers the database options that are available for your AquaChem project.

The following sections explain the menu commands in detail.

3.1 File Menu

New

The **New** option is only available when no other database is open. In order to activate this option, you must first close any database files which may be open.

The **New** command creates a new empty database based on a database template. The template is an empty database that contains all necessary data tables, parameters,

settings, etc., but does not contain sample or station data. When you create a new database, the database template is copied to the specified filename and location. Choosing a database as a template simply means that you will find the same Lookup-tables, Sample/Station Parameters, and Settings in the database as there are in the selected template.

The AquaChem directory contains two default database templates:

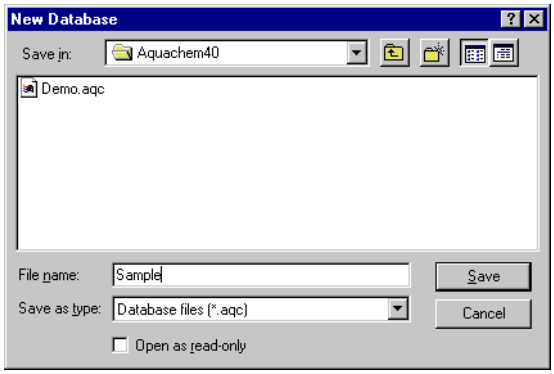
- **Template.TPL** is normally used to create a new database file.
- **Template.37** is used when opening a file from AquaChem version 3.7.

AquaChem lets you use any valid AquaChem 4.0 database as a template.

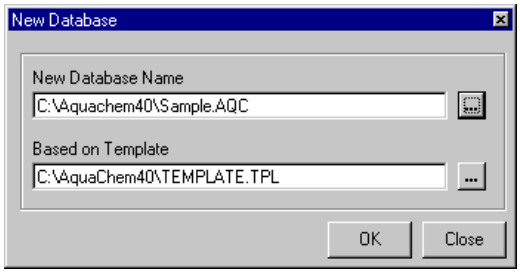
Creating a New Database

Follow the steps below to create a new AquaChem database file:

- Start AquaChem and press **[Cancel]** when prompted to open a database. (Or if you already have AquaChem opened, close the current open database by selecting **File > Close**.
- Select **New** from the **File** menu, and the **New Database** dialogue will appear as shown below.



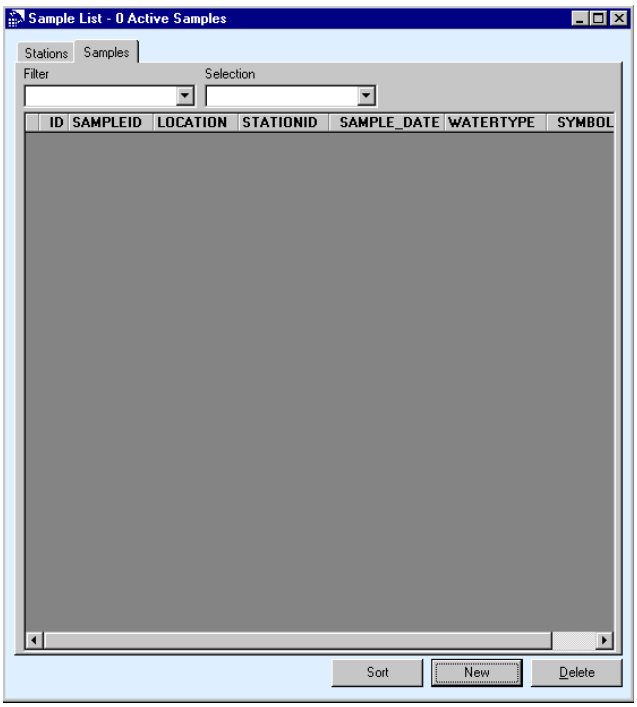
- Browse to the appropriate folder. The default folder is the installation folder C:\AquaChem40.
- Type in the name of the new database, and click **[Save]**.
- You will then see the following **New Database** dialogue.



- Below the database filename, you must specify a **Database Template** to use for the creation of your database. By default, AquaChem will use the **Template.TPL** file which is included with your installation. This template contains the same data structure as the demo database. When you first start using AquaChem, this will be the only database template file available, and in most cases this template file should be adequate. If you have other database templates available, click the ... button to browse and select a .TPL file to be used for your project.
- Once you are finished entering the .database (.AQC) and template (.TPL) name, press **[OK]**.

NOTE: Database filenames should be a combination of letters and numbers only. The filename and directory path should NOT contain spaces, accents, or other characters.

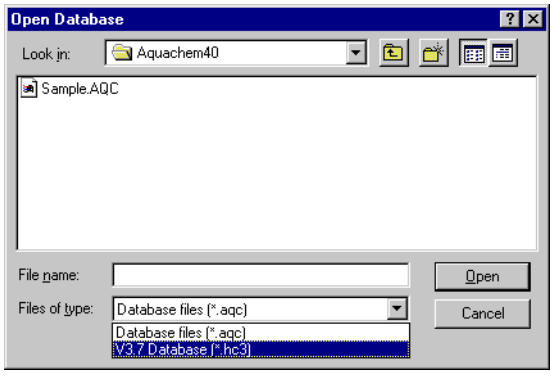
AquaChem will then automatically create a blank database file (with .AQC extension) using the associated database template file containing the data structure for each record in the database. An example is shown below:



If you use the Template.TPL file, then your data structure may contain some parameters which do not apply to your data set, while others may be missing. Use the **File > Database** options to modify the available parameters in the template. The database options are explained later in this chapter.

Open

The **Open** command opens an existing AquaChem database. When you select this command, the following dialogue should appear:



You may open either an .AQC (AquaChem database file) or an AquaChem V3.7 Database (*.HC3) file. When opening an AquaChem V3.7 file, the binary file (*.HC3) is automatically converted to an .AQC file.

NOTE: You may open a database which resides on a network computer. However, only one user should access a database at a time. Future versions of AquaChem will support Network Multi-user access of the same database file.

After you have selected the desired database, click **[Open]** to load the file into AquaChem. You may also open a database by picking the file from the recent file list, under the **File** menu.

NOTE: When opening an AquaChem v 3.7 database, ensure that all settings files reside within the same folder as the .HC3 file; this includes plot configurations (.GRF) and table settings (.RPT) files.

The **Open** database option is only available when no other database is open. In order to activate the Open command, you may need to first select **File > Close** to close the opened database.

Close

The **File > Close** command will close the current database. This will allow you to open other databases, or create a new database.

Save as Template

This option allows you to save the current database settings to a database template (.TPL) file. These settings can be used when creating future databases.

The **Template.TPL** file is used only in the initial step to create a database. Similar to a word template which you use to create a new word document, the document is completely independent of the template after the document is created. The same thing occurs with AquaChem; after the database is created, the Template file is no longer needed. You may add, remove, or change parameters and properties; all properties are stored in the .AQC database itself.

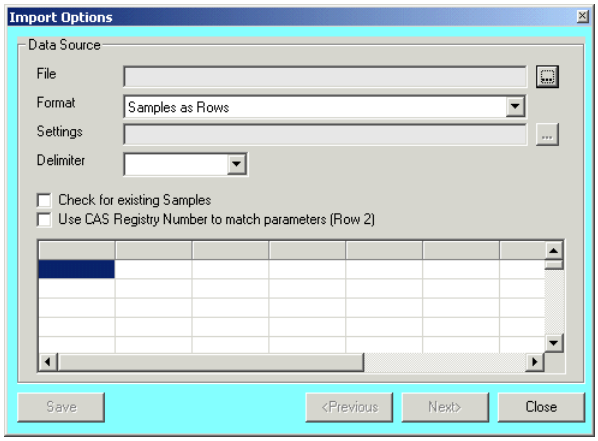
The **Save as Template** command is only available when a database is open, and the Active List window is active.

Save Database

Saves the database, or allows you to save the database under a different name and directory. The database file is saved with the extension .AQC.

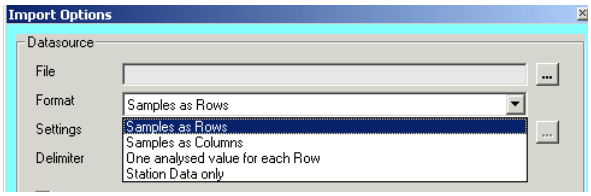
Import

The import option allows you to import **Sample** and **Station** parameter data into your AquaChem database. This option is only available when the sample/stations list window is the active window. The Import routine is separated into four simple steps. When you select **File > Import** from the main menu, the following dialogue will appear:



The source data file must be a text file with the data separated by a tab, semicolon, or comma. As such, the file extension must be .TXT, .PRN, or .CSV. If your dataset was created in a spreadsheet, use the **File > Save As** command in your spreadsheet program to save your data set as one of these file types. When using a character other than a tab (e.g. a comma or semicolon), ensure that this character does not exist in any of the text fields in the file. To load the data file, simply press the ... button beside the **File** field.

The file format is specified beside the **Format** field. Use the combo box (as shown below) to select the appropriate file format. The source data file may have the following four formats:



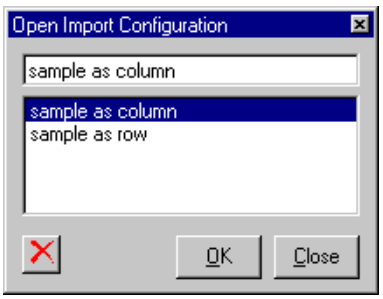
- **Samples as Rows** - this format requires the first row of data to have the parameter labels (one per column), and each new row is a new sample.

- **Samples as Columns** - this format requires the first column of data to have the parameter labels (one per row), and each new column is a new sample.
- **One analyzed value for each Row** - each new row contains new measured values (parameters are listed column wise)
- **Station Data only** - import just the Station Description fields. The first row contains station parameter labels, and each new row is a new station.

The first format **Samples as Rows** is the most common and more compact (where samples are rows, and parameters are as columns). The second format is commonly used with laboratory analysis results. This allows you to specify more data per analyzed parameter such as the MDL (minimum detection level), the method and the precision. This is not possible in the spreadsheet format, since every value must fit in one cell. The **Station Data Only** format will allow you to import just station parameters, such as X, Y, Z location, Station Name, location, well depth, etc. This allows you the option of importing the Station Description information once; after all of the stations are present, you need only to provide the StationID for all of the samples that are subsequently imported. If you select this option, each station must be in a separate row.

NOTE: Your data source file should not contain any units for the respective parameters.

The next line in the **Import Options** dialogue is **Settings**. This option allows you to use previously defined import settings. This is useful for importing data sets with similar formats. If you do not want to use import settings, then leave the settings field blank. If you want to use previous import settings, press the ... button to load a list of import configurations:



Select a configuration from the list, then click **[OK]**. If you do not have available import settings saved, then click **[Close]**.

The next step in the **Import Options** dialogue is to specify the **Delimiter** for the file. The Delimiter options are available in the combo box and can be **Tab**, **Semicolon**, or **Comma**. Choose the appropriate delimiter for your file. Once the correct delimiter is selected, the data preview window in the lower section of this dialogue should show a correct preview of your file.

The import routine has an option to **Check for existing Samples**; this will allow to add data to already existing samples in your database. When this option is enabled (checked), AquaChem will check for existing SampleIDs in your project database, and if an identical SampleID is found in the database, the import data will be written to the corresponding sample. If the import field includes data which is already in the database, the data in the database is automatically overwritten. This feature is useful, if data for

the same dataset has been analyzed by different labs and must be imported from different source files. If the **Check for existing Samples** option is unchecked, every record in the import file will create a new sample in the database, regardless if an identical SampleID exists or not. Please note that this may lead to duplicate samples being created in your project database.

AquaChem also provides you the option to identify and match **CAS Registry numbers**. If this option is enabled, AquaChem will use the CAS Registry number rather than the parameter name to match parameters from the import file to the database. In order to use this feature, the second row of the import file must contain the CAS registry number or the second column depending on the structure of the import file. Also the registry number must be specified in the database parameters. This feature is useful if the import file contains many organic contaminants, which often are written differently, and the parameter match between the database and import file is not very reliable. The CAS Registry number is unique and therefore all parameter matches are effectively realized. If you do not have CAS #'s in your file, then leave this box unchecked.

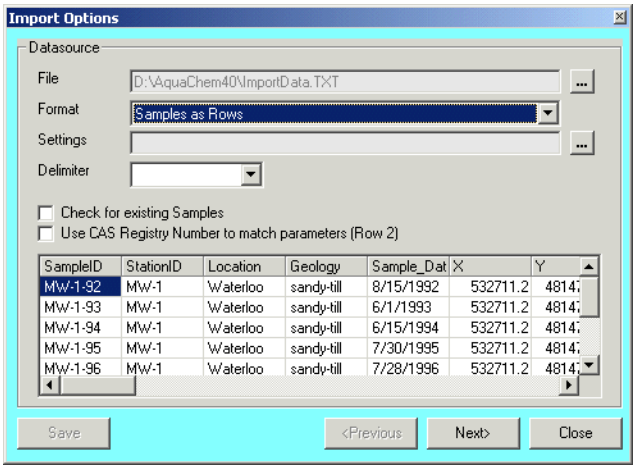
Example

To import a data file into your AquaChem database, please follow these steps:

Hint: Before proceeding with the import option, you should ensure that your source file containing your water analysis data is properly formatted. For your convenience, an Excel template is provided with AquaChem, which includes some of the most common sample and station parameters. This file is called **Import_Template.XLS** and can be found in your AquaChem installation folder. If you wish, you may use this file for your data set. Simply enter your data, then save the Excel file as "Tab-Delimited Text", and proceed with the import options. Or, you may use the ImportData.txt file as a guide; this file is also included in your AquaChem installation folder.

Step 1: Data Source File

- If you have not already done so, select **File > Import** from the main menu.
- Press the ... button beside the **File** field to locate the source file.
- Browse to the appropriate folder to locate your text file then click **[Open]**.
- Your filename should now appear in the **File** field, and a preview of the file should appear in the lower section of the dialogue.
- Select the import **Format** for the source file (Samples as Rows or Samples as Columns, etc.). For this demonstration, the **Samples as Rows** mode will be used.
- Choose the **Delimiter** for the source file.
- Enable or Disable the option to **Check for existing Samples**.

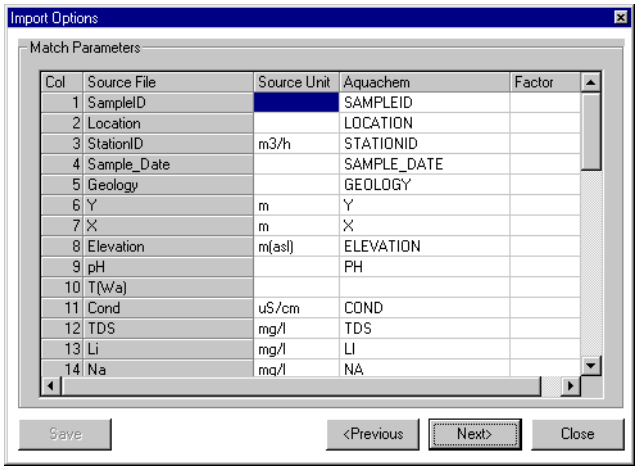


- Once you have entered the necessary details in the first import options dialogue, press the **[Next>]** button to proceed.

Step 2: Match Parameters

The next step in the Import data options is to Match Parameters.

The **Match Parameters** frame contains a table listing the Column numbers, the Source text file headers, the Units in the text file, and corresponding AquaChem parameter Internal Key values, as shown in the following **Import Options** dialogue.

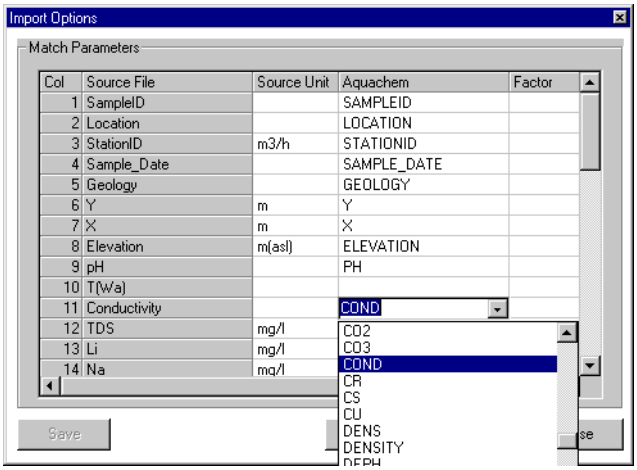


The **Source Unit** field is used to select a ‘default’ concentration unit for the imported parameters. If the unit is different in the import file and the database for the same

parameter, the import routine transforms all concentration values using the database units. (For example 10 ug/L Cu will become 0.01 mg/L Cu in the database).

There is also an option to apply a multiplication **Factor** to the incoming data set. A multiplication factor is needed if the species for the same parameter do not correspond. For example, if Silica is expressed in the import file as mg/L Si and as mg/L SiO2 in the database. In order to calculate the transformation factor for the respective species you may use the **Species Converter**, available in the **Tools** menu.

In this dialogue, you are required to match up the data in the source file to the appropriate AquaChem parameter labels. If there are blank fields in the AquaChem column, then this means that no match parameter was found in the database. This may be due to the lack of this parameter in the database, or that the parameter is written differently in the Source file. If the cell stays empty, the respective parameter will not be imported. For example, if your text file had the parameter name **Conductivity**, you must match this up to the AquaChem parameter Internal Key name **COND**. Blank fields must be linked manually using the steps below:



- Double-click in the grid cell under the **Aquachem** column and a combo box will appear listing all of the available parameters in your AquaChem database.
- Select the appropriate parameter to match to the import **Source File** column. This will correctly link the parameters in the source file to the parameter names in the AquaChem database template.
- Repeat this step for each parameter in your source file which has not been correctly mapped to an AquaChem database parameter.

HINT: If the field names in the text file are identical to the field names in the AquaChem database template file, the parameters will be mapped automatically to the AquaChem column. Therefore, if you format your

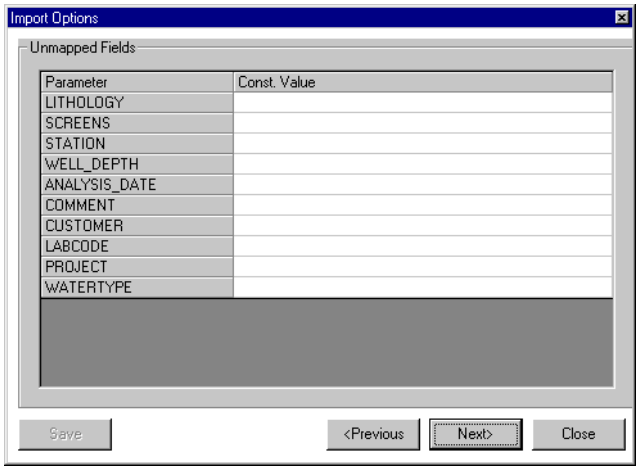
source file correctly prior to importing, you can save some time in this step.

AquaChem allows you to select variable concentration units for selected chemicals. Unless otherwise specified, the units used for that parameter will be identical to those specified in the database parameters options (under **File > Database**). To change the default units, double-click in the corresponding grid cell under the **Units** column and you will see a selection of available units (g/L, meq/L, mg/L, mmol/L, mol, ppm, umol/L, ug/L). Select the desired unit, and repeat this for other parameters as needed.

Once you have mapped all units and parameters, press the **[Next>]** button to proceed. If the data does not appear to be correct, press the **[<Previous]** button to return to the previous step.

Step 3: Unmapped Fields

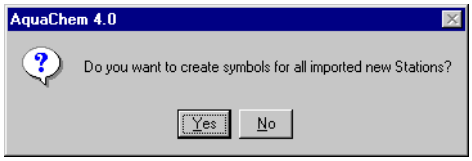
The next dialogue contains a list of the AquaChem parameters which were not matched up to parameters in the source file (ie. **Unmapped Fields**).



This dialogue allows you to enter constant values for these unmapped parameters; this is optional. For example, if all of the imported samples belong to the same project or the same location you may fill the respective fields automatically during this step of the import. To skip this step, leave these fields blank.

To proceed to the last step in the import routine, press the **[Next>]** button. To return to the previous step, press the **[<Previous]** button.

Upon proceeding, you will then see the following warning prompt:



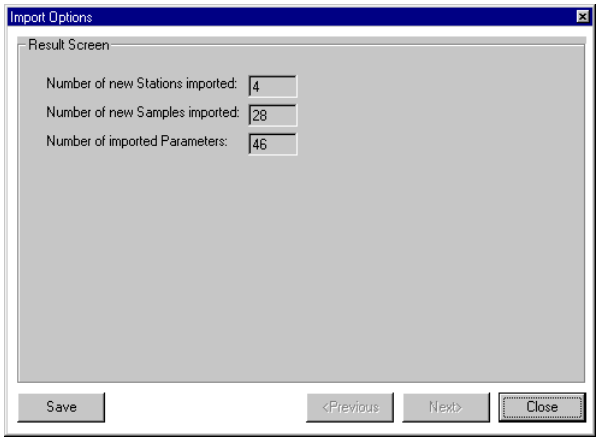
This option allows you to automatically create one symbol for each unique station in the imported source file. These symbols will be created in the Station symbol group. This is a very help feature, which can aid in plotting your sample data later on.

☞ **[Yes]** to accept this feature, or **[No]** to ignore this option.

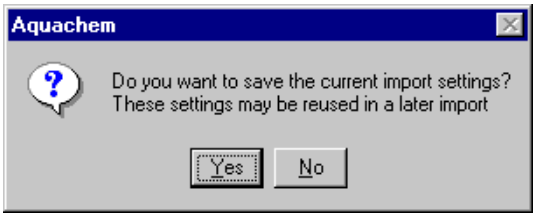
Step 4: Result Screen

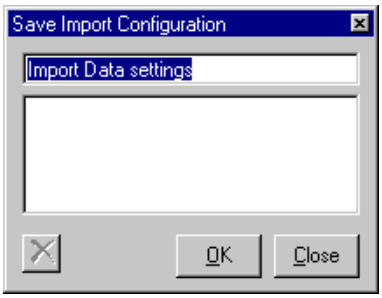
The last dialogue in the Import options is a summary of the results of the data import.

The **Result Screen** dialogue shows the Number of new Samples and Stations that were successfully imported, and the Number of parameters that were successfully mapped and imported.



Once you are finished, press the **[Close]** button. Upon closing, you will receive the following prompt:





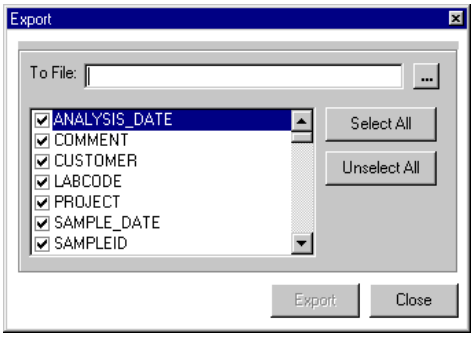
This option allows you to save the import settings (file format, mapped parameters, units, factors, and constant values) to be reused in the future. Click **[No]** to ignore this option. Or click **[Yes]** to save these settings and you will be prompted with a **Save Import Configuration** dialogue as shown on the right hand side. Simply enter a name for the import configuration, click **[OK] and then [Close].** After successfully importing the data, you will return to the main database window showing your active samples and stations. This concludes the necessary steps for importing data.

Export

The **Export** option allows you to export the data for active samples and stations, to a text file for use in other applications or in **Visual MODFLOW**. The **Export** command is only available when the Active List window is the current active window.

Text File

To export your sample/station data:

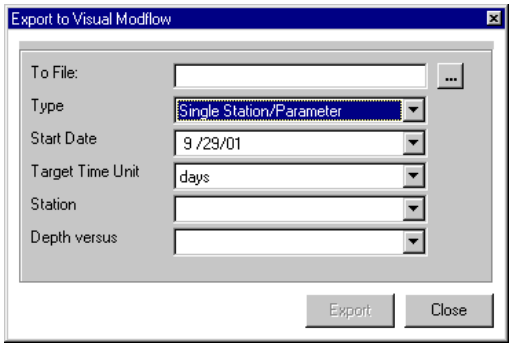


- Select **Export > Text File** from the main menu.

- Press the ... button to choose a filename for the file being exported.
- By default, all the parameters are selected and will be exported. The selected parameters are indicated by the presence of a checkmark beside the parameter name.
- To remove parameters from the export, remove the checkmark beside the parameter.
- To add all parameters to the list, press the **[Select All]** button.
- To de-select all parameters, press the **[Unselect All]** button.
- Once you are finished, press the **[Export]** button. A text file will be generated in tab- delimited format.
- Press **[Close]** to return to the main AquaChem window.

Visual MODFLOW

The **Export > Visual MODFLOW** option will export your current sample and station data to a space-delimited text file. The data can then be used for the input (concentration observation well data) of a Visual MODFLOW groundwater model.



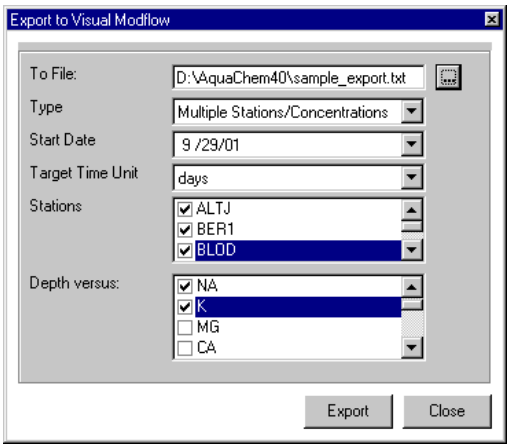
To export the data:

- Select **Export > Visual MODFLOW** from the main menu.
- In this dialogue, you must enter a filename, select the Export format, enter a Start date, Time unit, Stations, and Parameter. The default file type is **Single Station/Parameter**, however you can choose **Multiple Stations/ Concentrations** as well.
- If you choose the first type, the format of the file is as follows:

Each line has a time measurement and an observed concentration for a single parameter. The start date is used to calculate the time for the first observation.

NOTE: The **[Export]** button will become active only after the necessary options have been specified.

- If you choose **Multiple Stations / Concentrations** format, then the dialogue shown below will appear:



This format is only practical if a **Depth** parameter value is available in your database. If so, then select the stations you want to export, by placing check marks in the appropriate boxes. Then, beside **Depth versus,** place check marks beside the desired parameters that you want to export. After doing so, the observation name is concatenated with the station code and depth, in the resulting text file.

Once you have specified the necessary settings, press the **[Export]** button to proceed and generate the export file. Press the **[Close]** button to close this dialogue and return to the main AquaChem window.

Print

The **Print** command will load the print options for the current AquaChem window or dialogue. The print icon in the toolbar serves the same purpose. The **Print** option is only available when one of the following windows is active:

- Plots
- Tables (Spreadsheet View), or
- Reports

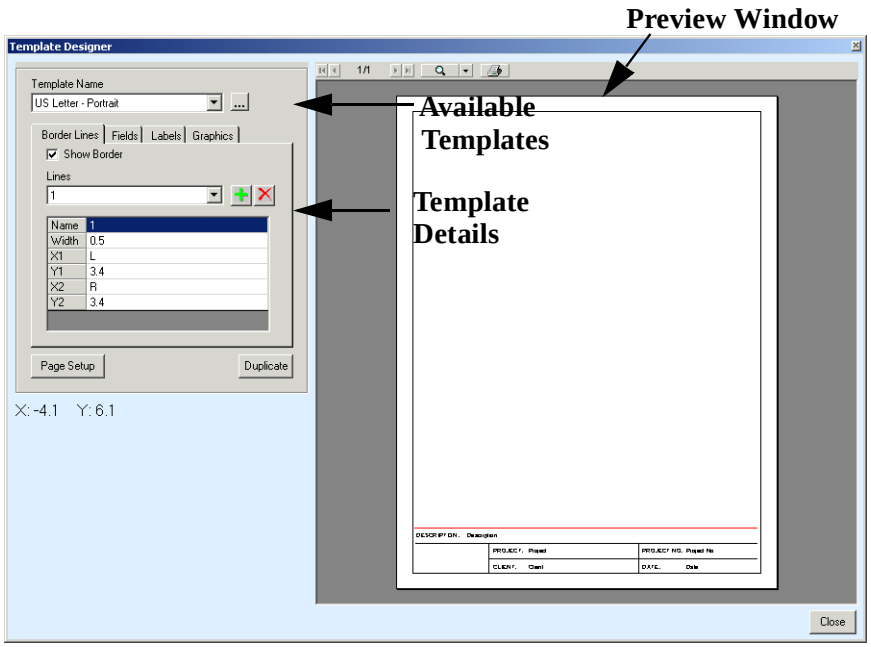
Please refer to Chapter 4: Printing and Exporting Plots for more details.

Template Designer

If the pre-defined printing templates built into AquaChem are not satisfactory for your needs, you can easily create your own customized printing templates using the **Template Designer**. The template designer option also allows you to duplicate and modify existing templates.

Template Designer Interface

When you select **Template Designer** from the **File** menu, the following dialogue will appear:



The **Template Designer** dialogue has three main components:

1. **Available Templates** in the upper-left corner containing the **Template Name** and a combo box listing the available templates.
2. **Template Details** is located immediately below the **Template Name** field. This includes the controls and tools for designing templates, such as:
   - **Border Lines**,
   - **Fields**,
   - **Labels**, and
   - **Graphics**
3. **Preview Window** on the right side of the dialogue, containing a preview of the Template as content is added or modified.

The options in the **Template Designer** allow you to:

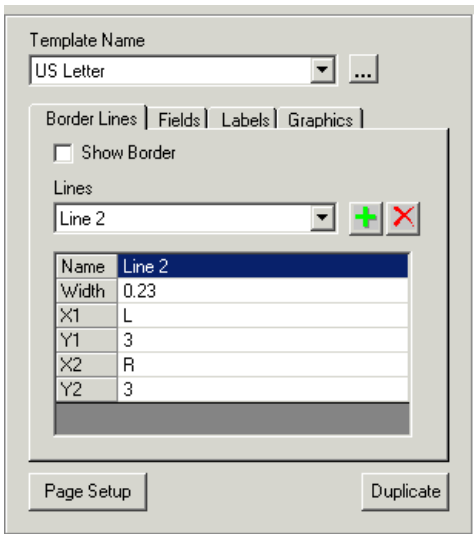
- Select the page size, orientation, and margins

- Draw lines and borders
- Define and position text block descriptors
- Position user-entry fields
- Add headers and footers, and
- Position and size bitmap graphics for a company logo

The following section provides more details on the functionality of the template designer.

Template Designer Controls

The main controls and tools for the **Template Designer** are on the left side of the main dialogue (as shown in the figure below).



At the top of this frame, you will see a list of the available templates; you can select a different template from the combo box. AquaChem includes the following pre-defined templates:

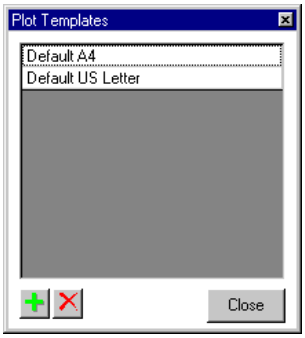
- US Letter - Portrait
- US Letter - Landscape
- A4 - Portrait
- A4 - Landscape

In the **Template Designer** dialogue:

- Click  button to add a new item to the template.
- Click  button to delete the currently highlighted item.

Note that the buttons are common to each tab. For example, if you are in the **Border Lines** tab and you press the  button, a new border line will be added. You can then proceed to enter the appropriate properties for this line in the fields below.

The  button in the **Template Designer** dialogue will load a **Template Name** dialogue as shown on the right. It displays the full list of templates currently available and will allow you to create and name new templates.



In the **Template Name** dialogue:

- Click  button to create a new template
- Click  button to remove an existing template

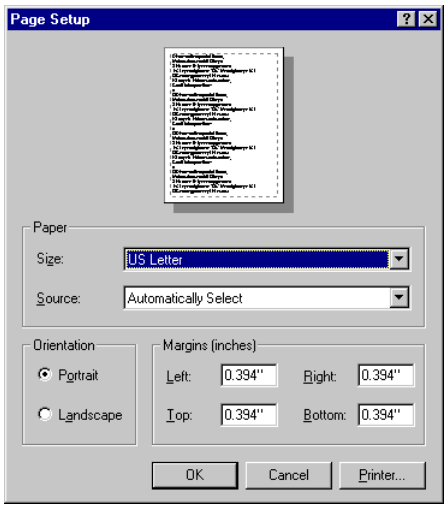
To rename a template simply place your mouse cursor in the appropriate field, then enter a new text label. Once you are finished in this dialogue press **[Close]**.

When positioning a line, field, or graphics, the X, Y page coordinates displayed in the lower left section of the main **Template Designer** dialogue can be helpful. These coordinates correspond to your mouse cursor location and can help you in the placement of starting and end points.

The **[Duplicate]** button will duplicate the currently selected template. The duplicate template will be named **Copy of TemplateName**, and the duplicate template will have the same layout and characteristics as the originally selected template. If it is your first time creating or customizing a Print Template, it may be easier to modify a duplicate copy of an existing template, than to start from the beginning. Please note that each Template must have a unique name.

NOTE: Although you have the option of modifying the default template designs, it is strongly advised that you either duplicate the selected template, or create a new blank template. This avoids damaging or losing the original template designs and ensures you will always have a standard set of default Print Templates.

When you press the **[Page Setup]** button, the following **Page Setup** dialogue will appear:



In this dialogue, in the upper **Paper** section you can define paper **Size** and **Source**.

In the lower **Orientation** section, you can define paper orientation and page **Margins** for the template. The page margins will correspond to the location of the page border. The page dimensions inside the margins will be used to automatically locate and size the selected plots.

You can also access your standard Windows Printer options by pressing **Printer** button. Once you are finished, press **[Cancel]** to return to the previous dialogue.

Creating New Templates - Example

The following section describes the options of the **Template Designer**, and how it can be used to build and customize your own templates. The brief instructions below tell you how to create a basic printing template, and how to customize this to your own preferences.

- Click ... button to load the list of Templates.
- Click + button to create a new template.
- Enter a name for the new template (e.g. “Sample-Letter” for these instructions).
- Press **[Close]**.
- Choose this template from the combo box.

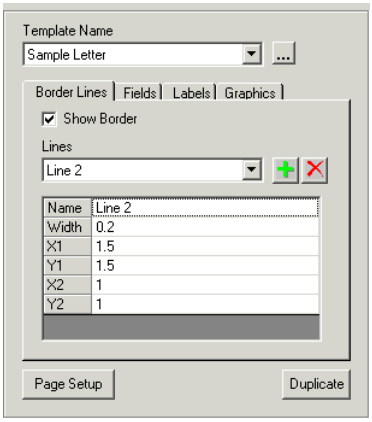
You will then see a new blank Print Template in the preview window. By default, all new templates include a border and default page settings.

Creating Border Lines

The first tab in the template designer dialogue is **Border Lines.** This tab allows you to create the Print Template form by drawing lines indicating the borders of the template Title Blocks. Each line has a **Name**, **Width**, starting coordinates (**X1**, **Y1**), and ending coordinates (**X2**, **Y2**). The coordinates units are in cm. The coordinates are measured from the origin, which is the bottom left corner of the page. The **Show Border** check box shows/hides a page border.

To create a new Line:

- Click + button and a new Line will be created with the name **#new Line.**
- Double-click in the **Name** field and enter a unique name for the new line (e.g. Line2).
- Enter a line **Width** 0.2.
- Enter the desired start and end coordinates for the new line (X1, Y1 represents the starting point of the line, and X2, Y2 represents the end point of the line). The bottom-left corner of the Preview Window serves as the origin for the Template designer.



To edit an existing line, select the line from the list and enter the new coordinates. For example, if you want to start a line at a point located 1.5 cm from the bottom of the page and 1.5 cm from the left side of the page, you would enter a line with X1 = 1.5 and Y1= 1.5 (cm). Remember that you can always use the mouse pointer to check the page coordinates, as shown on the left side of this dialogue.

If you want to enter line locations to coincide with margin locations, enter the following items for the X or Y coordinate:

Enter "**L**" to have a line coordinate equal to the **left** margin location.

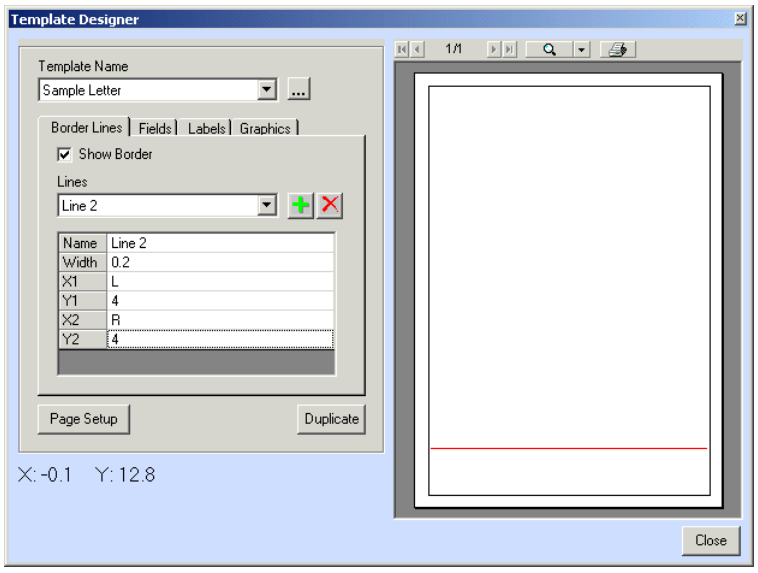
Enter "**R**" to have a line coordinate equal to the **right** margin location.

Enter "**T**" to have a line coordinate equal to the **top** margin location.

Enter "**B**" to have a line coordinate equal to the **bottom** margin location.

This is useful if you want the lines to automatically adjust as the page margins change. An example is shown below:

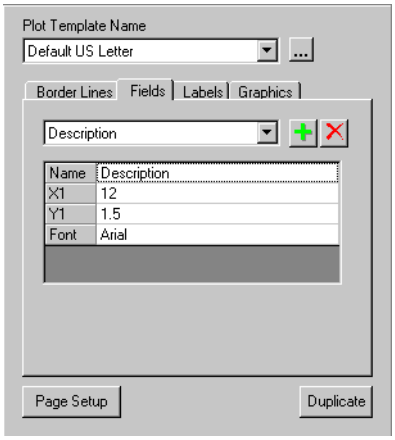
In this example, a line would be located at a height of 4 cm from the bottom of the page (Y1 and Y2 = 4) and the line would extend from the left page margin (X1 = L) to the right page margin (X2 = R) as shown below.



NOTE: To allow for quick recognition, the selected line, field or label is colored in **red** in the preview window. This will help you to quickly choose the starting and end points.

To remove existing lines, select the line then press the  button. The template designer settings will automatically be saved to the database; as such there is no Save button required in this dialogue.

Creating Fields



The next two tabs in the template designer are **Fields** and **Labels**. These provide options for adding text to the template. The fields tab is used to create, position and label the Text fields. Beside each field, there will be a corresponding label.

The Text fields are the items which will show up when you load the template into the print preview window, and will be blank and prompt you to enter the specific details.

To create a new Field:

- Click  button and a new Field will be created with the name #new Field.
- Enter a unique name for the field.
- Enter the appropriate page coordinates for the field (the position refers to the page coordinate location for the bottom-left corner of the field). Remember to leave room for the Label which will typically be placed to the LEFT of the field.
- Select an appropriate font for the field. Click once in this field, and you should see a  button will appear. Press this button to access the font options for this field.

To modify an existing field, select this item from the combo box, and make the desired changes to the position, text value and/or font. The  button can be used to remove existing fields from the template.

The next step is to create a **Label** for the Text Field. As mentioned above, the Label is commonly positioned immediately to the left of the Field, using the same Y-coordinates. Therefore, take note of the Y-coordinates for the field(s) you just created, so they can be used for the corresponding label.

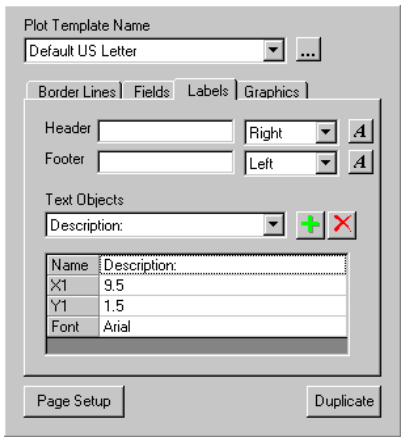
Creating Labels

The fixed text **Labels** are hardcoded into the template; this means that this item will always show up once the template has been selected, and will be Read-Only in the print options window. Beside each label, there is a **Field** entry, which receives the actual text entry for the printout when the template is loaded (information is entered into the fields in the print preview window).

For example, a label item would be Date; beside the date, there would be a Date field. When the template is loaded into the print options window, you will be prompted to enter a Date in the Date field, which corresponds to the plot or report(s) which has been selected for printing.

AquaChem allows you to specify multiple labels at any location on the page. These labels generally contain static project information such as **Client**, **Project** number, and **Date**.

The **Labels** tab allows you to create, position and customize the Labels on the template.



At the top of this dialogue, there are defaults for a **Header** and **Footer** for the template. The header position (**Left**, **Center**, or **Right**) can be adjusted along with the font (press the A button to access the font options for the Header or Footer). If you do not want a header or footer, simply leave this field blank.

In the lines below, you will see the list of labels.

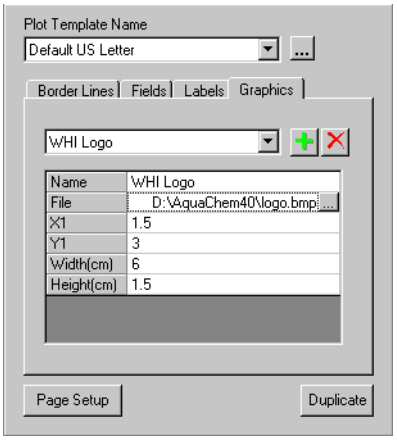
To create a new label:

- Click + button and a new Label will be created with the name #new Text.
- Enter a unique name for the label.
- Enter the appropriate page coordinates for the label. (X1, Y1 refers to the page position for the bottom-left corner of the label). It is common to position the label to the left of the corresponding field. If necessary, use the preview window as a guide.
- Select an appropriate font for the label. Click once in this field, and you should see a ... button appear. Press this button to access the font options for this label.

To modify an existing Label, select the item from the combo box, and make the desired changes to the position, text value and/or font. The X button can be used to remove existing Labels from the template.

Creating Graphics

The **Graphics** tab in the template designer dialogue allows you to import company logo graphics into the template design.



You may set the position of the image on the page and specify the size as it will appear on the page. Each of the default Print Templates has been designed to accommodate an imported bitmap image of your company logo or your client's logo (or any bitmap image). AquaChem currently supports only bitmap image files (filename.BMP) as the graphics format.

To import a new bitmap image file:

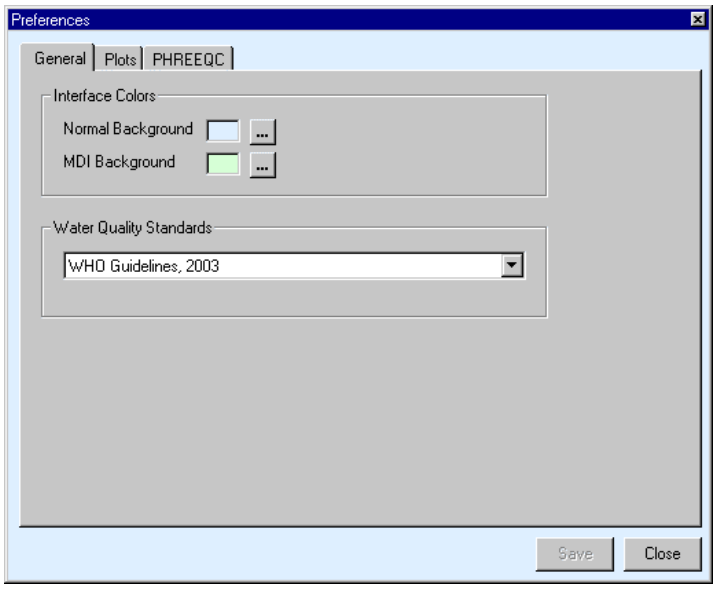
- Click  button and a new Graphics entry will be created with the name #new Picture.
- Enter a **Name** for the new graphics.
- Click once in the **File** field and a  button should appear. Click this button to browse the bitmap image file (filename.BMP) and then to import the image click **[Open]**.
- Enter the position coordinates of the bitmap (the position of the bitmap refers to the X-Y page coordinates for the top-left corner of the bitmap image).
- Enter the **Width** and **Height** of the selected bitmap file. The dimensions of the bitmap image refers to the Width and Height of the bitmap image as it will appear on the page. The bitmap image will be automatically re-sized (e.g. stretched or compressed) to fit the dimensions.

To modify an existing bitmap file, select the graphics from the combo box, and make the desired changes to the position, name, position or dimensions. The  button can be used to remove existing bitmap logos from the list.

This concludes the steps for creating Print Templates.

Preferences

The **Preferences** dialogue loads the general user preferences for AquaChem. These can be accessed only when the sample/station list is active. This dialogue contains three main tabs: **General**, **Plots** and **PHREEQC** as shown below. A detailed description for each of these tabs is provided in the following section.



General

The above figure is a screen capture of the **General** tab. It is used to control the Interface Colors and to specify the Water Quality Standards, as described below.

Interface Colors

In the **Interface Colors** dialogue, you can specify the AquaChem **Normal Background** and the **MDI** (Multiple Document Interface) **Background** colors. Simply click on the ... button and a standard windows **Color** options dialogue will load allowing you to choose another color.

Water Quality Standards

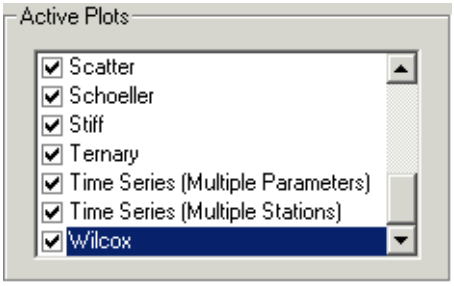
In this frame, you can specify the set of **Water Quality Standards** to be used for the current database in AquaChem. Aquachem 4.0 allows you to define multiple guideline levels, however only one set can be used at one time.

The data for each Water Quality Standard is specified in the **Database** dialogue which can be accessed through **File > Database > Water Quality Standards.** In here, you may edit existing values for the standards for each parameter. You can also create your own set of Water Quality Standards and import or manually enter values for these new standards.

Plots

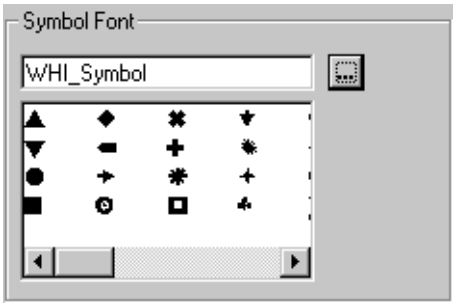
The second tab in the Preferences dialogue contains settings for **Plots** which is used for the settings in the Plots and Symbols.

Active Plots



The upper left frame of this dialogue lists the **Active Plots**. This allows you to activate / deactivate the plots which appear in the **Plots** menu (main toolbar). Active Plots are indicated by the presence of a checkmark beside the plot. By default, all plots are active.

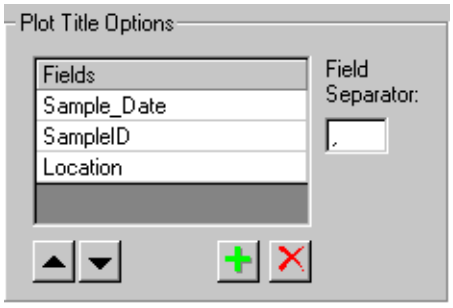
Symbol Font



In the upper right frame of this dialogue you will see options for the **Symbol Font**. AquaChem now uses “True type fonts” for symbols on plots and graphs. As such, there is an unlimited number of symbols that you can use for your project database. The default font selection is **WHI_Symbol**. To choose another font type, press the ... button.

NOTE: The symbols can be defined through the main menu: **Plots > Define Symbol or Line** dialogue.

Plot Title Options

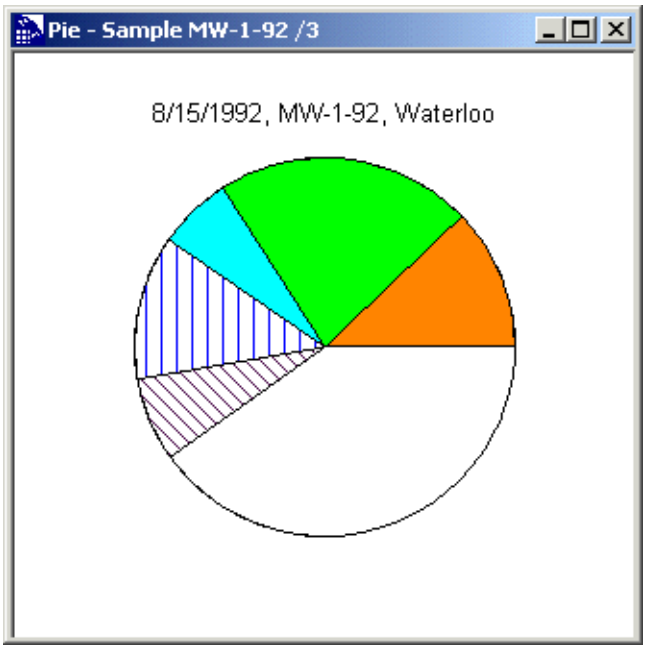


This frame includes settings for the automatic plot titling option. When a new **Pie, Radial,** or **Stiff** plot is created with your samples, the plots will automatically be titled with the descriptive fields (parameters) listed here. You can specify which parameters you would like to be utilized when using the automatic title option.

To do so, click the + or × button to add or remove parameters. To change existing fields, simply double click in the field and choose a new parameter from the combo box. The parameter order can be arranged using the up and down buttons. Once you are satisfied with the parameters, you must specify a **Field Separator**. This will be the character that

separates the parameters in the title of the plot. You can use any character as the field separator, however the most common are a hyphen, a comma, or a semi-colon.

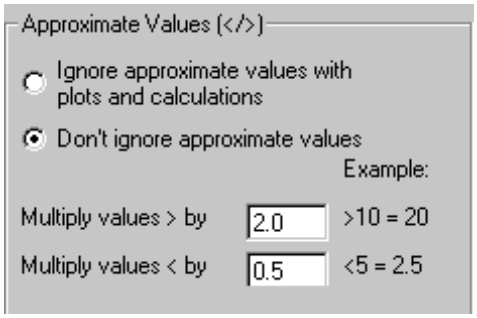
Based on these preferences, all new Pie, Radial and Stiff plots will be titled with the unique descriptive parameters for the individual sample. Using these parameters above, you can see an example of a Pie Plot which is created with the automatic title option.



The title of the Pie plot uses SAMPLE_DATE (8/15/1992), SAMPLEID (MW-1-92), and LOCATION (Waterloo), separated by a comma.

Approximate Values [</>]

In the right frame of the preferences dialogue, you have options for displaying data with approximate values. AquaChem allows you to enter and store approximate measured values using the less than (<) and greater than (>) symbols. The approximate values option requires you to specify whether the approximate values will be ignored or included in the plots.



- If you choose to **Ignore approximate values with plots and calculations**, they will be treated as null entries.

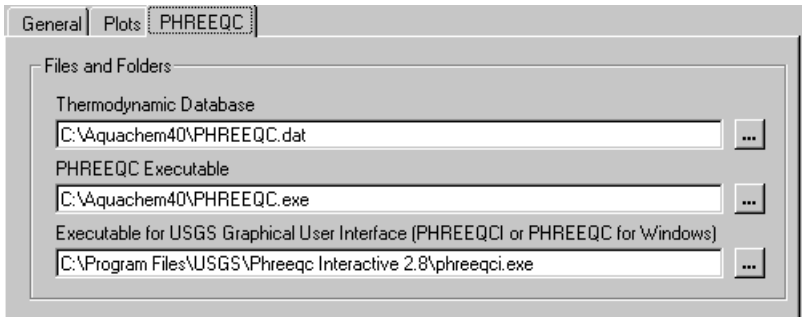
- If you choose **Don't ignore approximate values**, you may specify by which factors <> these values are multiplied for the use in plots or calculations. For example, if 2.0 and 0.5 are specified, a value of >10 will be taken as 20, and a value of <5 will be taken as 2.5.

PHREEQC

The last tab in the preferences dialogue has options for **PHREEQC**; this controls specification of PHREEQC related Files and Folders.

Files and Folders

In this dialogue (shown below), you must specify the locations of the PHREEQC **Thermodynamic Database** (phreeqc.dat) and the **PHREEQC Executable** (phreeqc.exe) files. These files are required for running PHREEQC simulations.



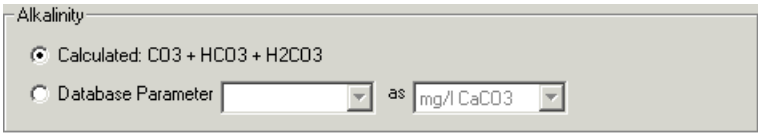
Under the **Files and Folders** frame, press ... button beside the **Thermodynamic Database** field and select the path and filename from the **PHREEQC Thermodynamic Database** dialogue. From this dialogue, select either **phreeqc.dat**, **Wateq4f.dat** or **Minteq.dat**. In addition, in the **PHREEQC Executable** field select the path and filename for the **phreeqc.exe** file. Finally, specify the path and filename for the USGS PHREEQCI.exe file (or the PHREEQC for Windows executable, if this component is installed). To change the directories for these files, press the ... button beside each directory path, and specify the new file/folder location.

By default, all PHREEQC input and output files will be saved in your AquaChem installation folder (default is C:\AquaChem40).

Once you are finished, click **[Save]** then **[Close]**. You are now ready to run PHREEQC.

Alkalinity

There are two options for calculating alkalinity for use in PHREEQC:



- Alkalinity is **Calculated as the sum of CO3, HCO3, and H2CO3**; OR
- Alkalinity can use a measured **Database Parameter**. Simply choose a parameter from the list of available parameters and specify the desired units. The units may be °f, °g, mg/L CaCO3 etc.

Database

The **File > Database** command loads the AquaChem database options for your current database. This option is only available when the active list is the current window. For details on the **Database** options dialogue, please refer to **The AquaChem Database** section at the end of this chapter**.**

Exit

The **Exit** command will exit AquaChem. Ensure that all changes are saved to your database before exiting the program.

3.2 Edit Menu

The Edit menu provides access to commonly used Windows tools such as **Copy**, **Paste**, and **Cut**. The Copy, Paste and Cut commands are not available when the active list window is the active window; these options are only available when you are viewing or editing data for a sample or a station.

Copy

Copies the selected data or plot to the Windows Clipboard.

Paste

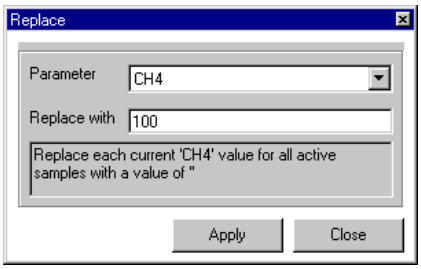
Pastes data from the Windows clipboard into the selected field. In order to paste numerical values into a sample details field, the field must be active, which is indicated by a flashing cursor in the field. Simply double click in the appropriate field, and field will become and active, and will be ready to accept data from the clipboard.

Cut

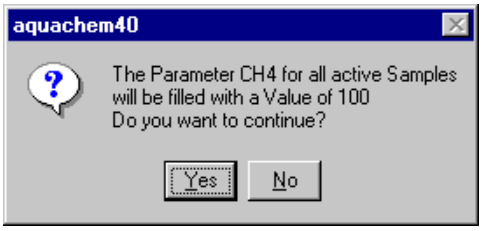
Cuts selected data.

Replace

The **Replace** command allows you to replace data for an individual parameter with a new value for all active samples in the database.



Simply choose a parameter from the combo box beside **Parameter**. Then enter a new value in the **Replace with** field. Once you are finished, press **[Apply]**. A warning message will appear as shown below to choose **[Yes]** to proceed or **[No]** to cancel the operation.

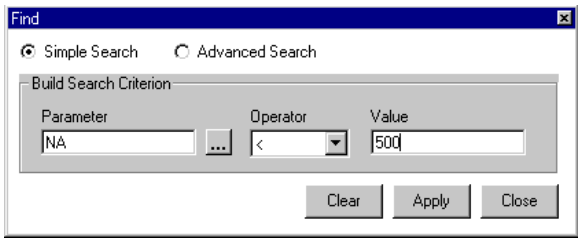


For the data entered in the above dialogue box, choosing **[Yes]** will replace all CH4 values for all active samples in the database with a new value of 100.

NOTE: The units for this parameter are based on the pre-defined units for the parameter, as specified in the database options.

Find

The **Find** utility is used to perform queries of the AquaChem project database. The Find dialogue allows you to create SQL-like queries of the samples or stations in the AquaChem database.



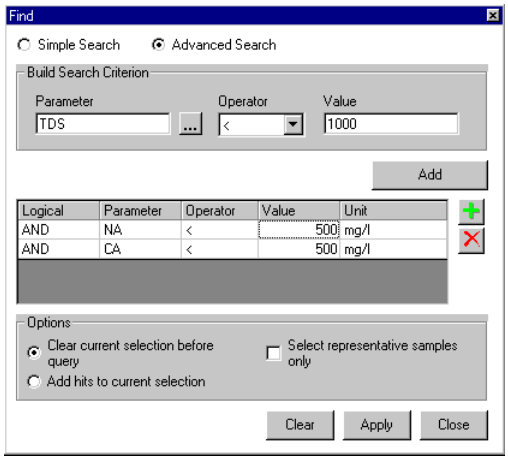
You may run a **Simple** or **Advanced** search. All found records matching the search criteria will be selected (highlighted) in the active list window after the search operation is completed. This feature is very useful for filtering the active list to include only those samples or stations which meet a set criteria.

To run a **Simple Search**:

- Enter a parameter in the **Parameter** field, or click ... button to select a parameter from the list.
- Select the desired **Operator** (<, >, =, LIKE). Searches for strings that use the = operator return exact matches, whereas searches that use the LIKE operator return matches that contain the substring you have specified in the **Value** text field. Searches for character strings are not case sensitive.
- Enter the corresponding parameter **Value**. (The units for the parameter value will be read from the Database options for the selected parameter.)
- Press **[Apply]**.

The records which satisfy this criteria will then be highlighted in your active list. You can now use the filter options in the active list to create and save the selected samples/ stations.

When you select **Advanced Search** the following dialogue will appear:



This option allows for a more advanced search of your database. It allows you to combine queries with logical operators, select the unit for each concentration parameter and to search on function results as well. (e.g. Find all samples where Cl <50 AND Hardness > 100).

To run an **Advanced Search**:

- From the top of the **Find** dialogue, select the **Advanced Search** option
- Enter a search string (**Parameter**, **Operator**, and **Value**)
- Press the **[Add]** button
- This will cause the search string to be moved to the lower half of this dialogue. You can now add an additional search string.
- Press **[Apply]** after you entered the desired search strings, to run the query.

The **Logical** field is a combo box containing 'AND' and 'OR'. These logical operators are used to link multiple search criteria. This field is only available after you have entered at least one search criterion. The **Parameter** field is used to specify a database parameter on which to base the query. Below the **Operator** field, there is a combo box listing the available comparison operators (>, <, =, and LIKE). In the **Value** field, enter a parameter value for the Find criteria. The **Units** field is used to select a unit system for searches based on chemical parameters.

The **[Add]** button is used to transfer the specified search criteria to the Search Criterion list box. You can also type the query expression directly into the Search Criterion text field if you are familiar with the format. The  and  buttons allow you to add or remove search strings directly to the search criterion frame.

Under the **Options**, you must specify the query options for the **Advanced Search**:

- **Clear current selection before query**: this will cause the current search query to be cleared, and run a fresh new query.
- **Add hits to current selection**: this will not remove active samples from the database.

The **Select Representative Samples Only** option will find only samples that fulfill the current query and are marked as representative in the Sample Details window. This might be useful when comparing samples for different sites and you only want to see a few representative samples per site on plots, reports, etc.

You can assign a representative sample for each site when entering the data in the Sample Details window using **Sample > Representative > On**. If you use the **Select Representative Samples Only** option, only the samples which are representative of each site, and which satisfy the search criterion are returned.

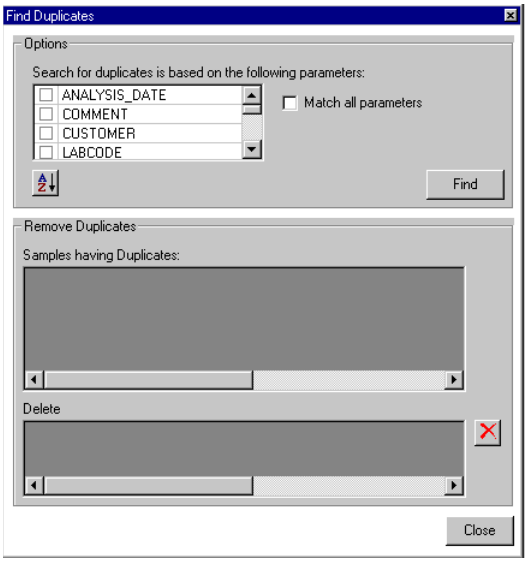
Below are a few examples of the Search Criterion and Search Results:

Date > 01.01.1960	Returns all records sampled after January 1st, 1960.
Location = Baden	Returns all records with location "Baden".
Location LIKE Baden	Returns all records with location containing the substring "Baden" (e.g. Baden, Badenweiler, Badentown, etc.)
Na/Cl>0	Returns all records with non-zero concentrations of Na/Cl (choose units of mmol/L when using ion ratios).

NOTE: The **Find** selection is context sensitive: if the **Samples** tab is active in the main list, the find will allow you to build and run a Find operation on samples; if the **Stations** tab is active, the find will be applied to stations.

Find Duplicates

The **Find Duplicates** utility allows you to find and remove duplicate samples or stations:



Simply choose a parameter from the list of available parameters by placing a check mark in the appropriate box. Only Sample Description and Station Description parameters are available. Or to select all parameters, place a checkmark beside **Match all parameters**. Then click the **[Find]** button.

AquaChem will then run a query on your database and locate all samples for which the values of the set of specified parameters are identical. Common parameters for this utility are site and date.

The results will then be shown in the lower half of this dialogue. Simply select on the samples you want to remove and press the  button to permanently remove these samples from your project database.

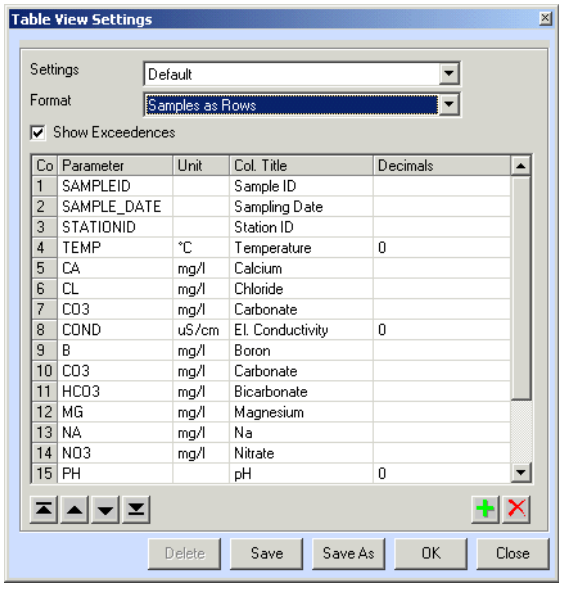
3.3 View Menu

Table View

AquaChem allows you to view and edit data in a tabular spreadsheet-like format containing all samples currently displayed in the Active sample list. This is a convenient method of handling a series of data or comparing selected parameter values for multiple samples. To create a spreadsheet view of the database, select **Table View** from the View menu. You can then use the **Create** option to create your own template or, view the **Default** table view or **Contaminants** view.

Create

When you select the **Create** option, a **Table View Settings** dialogue will appear (as shown below) listing the parameters that will be included in the columns of the spreadsheet. It is best to customize your spreadsheet first, before loading data into it.



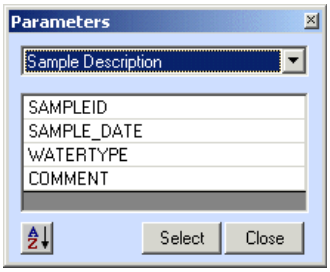
The **Table View Settings** dialogue can be used to select only those parameters you are interested in viewing/editing in a spreadsheet format.

At the top of this dialogue, in the **Settings** field, you will see the name of the current table.

The **Format** may be set to **Sample as Rows** (standard) or **Sample as Columns**; the latter gives a better overview if the spreadsheet contains only a few samples.

In the lower half of the **Table View settings** dialogue, you will see the list of parameters as they will appear in the table. The order of the parameters can be changed by using the top, up, down, and bottom arrow buttons (as shown here).

Parameters can be added or removed to the table view.

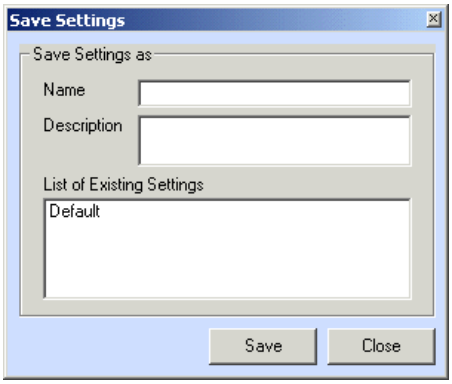


To add a parameter,

- Click the  button in the **Table View settings** dialogue and a **Parameters** dialogue will appear as shown on the right.
- Select the Parameter category by pressing the  button
- Choose parameter(s) from the list that appears
- Press the **[Select]** button.
- Press **[Close]** to return to the previous dialogue.

To delete a parameter(s), simply select parameter(s) from this list and press the  button.

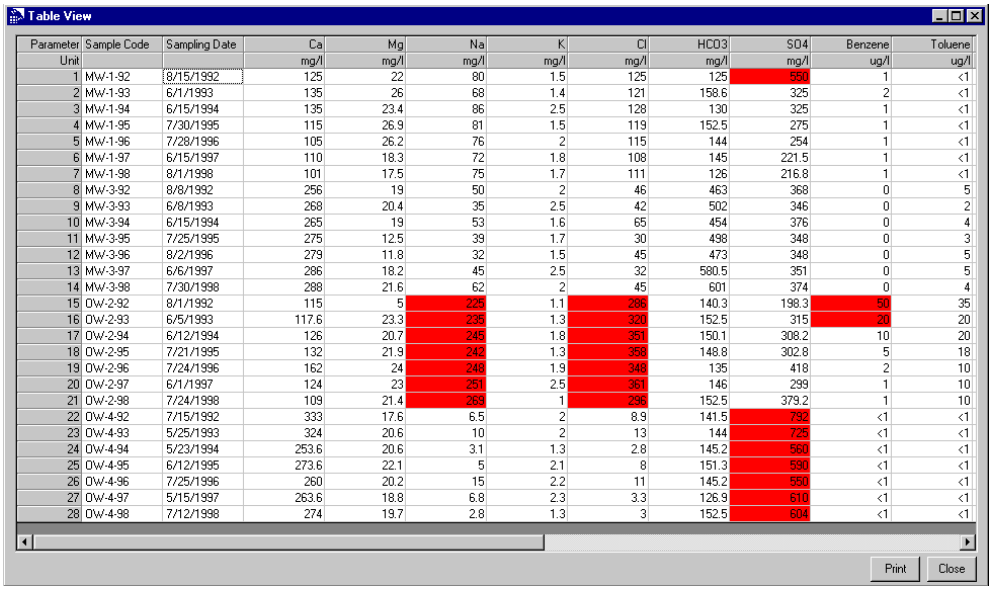
The **Unit** for the table view can also be changed, along with the column (**Col Title**) or row titles. Once you are satisfied with the Table view, press the **[Save]** button at the bottom of this dialogue. Alternatively, you may save the table view settings under a new name. To do so, press the **[Save As]** button at the bottom of this dialogue, and this will load the **Save Settings** dialogue as shown below.



In this dialogue, enter a **Name** and **Description** for the new Table View you have created and press **[Save]** to return to the Table View settings dialogue. Saved settings can now be retrieved from the **Settings** combo box of the **Table View Settings** dialogue. In addition, this new Table View will now appear under the AquaChem **View > Table View** menu below the **Default** table view.

Once you are finished, click **[OK]** to load the **Table View** window.

In the **Table View Settings** dialogue, you may activate the option **Show Exceedances**. When this option is enabled, clicking **[OK]** will display the **Table View** dialogue as shown below.



Parameter	Sample Code	Sampling Date	Ca	Mg	Na	K	Cl	HCO3	SO4	Benzene	Toluene
Unit			mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	ug/l	ug/l
1	MW-1-92	8/15/1992	125	22	80	1.5	125	125	550	1	<1
2	MW-1-93	6/1/1993	135	26	68	1.4	121	158.6	325	2	<1
3	MW-1-94	6/15/1994	135	23.4	86	2.5	128	130	325	1	<1
4	MW-1-95	7/30/1995	115	26.9	81	1.5	119	152.5	275	1	<1
5	MW-1-96	7/28/1996	105	26.2	76	2	115	144	254	1	<1
6	MW-1-97	6/15/1997	110	18.3	72	1.8	108	145	221.5	1	<1
7	MW-1-98	8/1/1998	101	17.5	75	1.7	111	126	216.8	1	<1
8	MW-3-92	8/8/1992	256	19	50	2	46	463	368	0	5
9	MW-3-93	6/8/1993	268	20.4	35	2.5	42	502	346	0	2
10	MW-3-94	6/15/1994	265	19	53	1.6	65	454	376	0	4
11	MW-3-95	7/25/1995	275	12.5	39	1.7	30	498	348	0	3
12	MW-3-96	8/2/1996	279	11.8	32	1.5	45	473	348	0	5
13	MW-3-97	6/6/1997	286	18.2	45	2.5	32	580.5	351	0	5
14	MW-3-98	7/30/1998	288	21.6	62	2	45	601	374	0	4
15	OW-2-92	8/1/1992	115	5	225	1.1	286	140.3	198.3	50	35
16	OW-2-93	6/5/1993	117.6	23.3	235	1.3	320	152.5	315	20	20
17	OW-2-94	6/12/1994	126	20.7	245	1.8	351	150.1	308.2	10	20
18	OW-2-95	7/21/1995	132	21.9	242	1.3	358	148.8	302.8	5	18
19	OW-2-96	7/24/1996	162	24	248	1.9	348	135	418	2	10
20	OW-2-97	6/1/1997	124	23	251	2.5	361	146	299	1	10
21	OW-2-98	7/24/1998	109	21.4	269	1	296	152.5	379.2	1	10
22	OW-4-92	7/15/1992	333	17.6	6.5	2	8.9	141.5	732	<1	<1
23	OW-4-93	5/25/1993	324	20.6	10	2	13	144	725	<1	<1
24	OW-4-94	5/23/1994	253.6	20.6	3.1	1.3	2.8	145.2	560	<1	<1
25	OW-4-95	6/12/1995	273.6	22.1	5	2.1	8	151.3	590	<1	<1
26	OW-4-96	7/25/1996	260	20.2	15	2.2	11	145.2	550	<1	<1
27	OW-4-97	5/15/1997	263.6	18.8	6.8	2.3	3.3	126.9	610	<1	<1
28	OW-4-98	7/12/1998	274	19.7	2.8	1.3	3	152.5	604	<1	<1

In this dialogue, the colored cells indicate sample exceedences, as defined by the currently selected Water Quality Standards (WHO, CCME, or US EPA). Samples which exceed the guidelines will be shaded with the appropriate color (red, orange, or yellow), as defined in the Database Options: **Water Quality Standards**.

You may edit the data in this window as needed; simply edit the required cells with new values. New data will be automatically saved to the database.

NOTE: You may not edit a cell displaying a station parameter. The reason for this is that the station parameters are not entered for each sample; instead each sample has a reference to the station table. Editing a station would edit this station in all samples where it is referenced. If you need to reference a different station for a sample, use the **Assign Station** option when you are in the Sample Details window **(Sample > Assign Station)**. If you need to assign a station that does not yet exist in the database, create a new station using the **Station > New** command.

You may print the table view by pressing the **[Print]** button at the bottom of the window, or select **Print** from the main menu.

Select **File > Save** from the main menu to save the table view; the file may be saved as a Text file (.TXT) or .CSV.

To return to the main AquaChem window, press **[Close]**.

Default

The **Default** command will load a default **Table View** with default parameter settings.

Contaminants

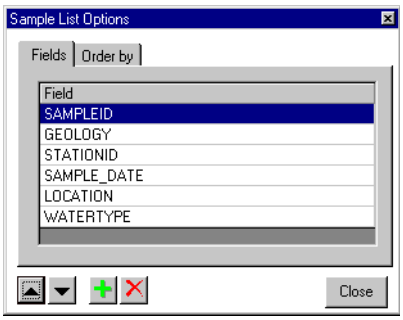
The **Contaminants** command will load a **Table View** with common contaminants.

Options

The **Options** command will load the options dialogue for the current AquaChem window. There are options available for the various AquaChem windows. The options will be different for plots, table view, active list and the Sample Details windows. Each of these is explained below.

Options - Active List

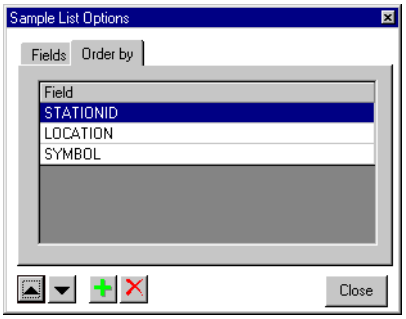
The active sample/station list can contain any sample/station description parameter from your database. To edit the parameters in the active list, select **Options** from the **View** menu (alternatively you can press the **[Sort]** button at the bottom of the active list window).



The first tab in the **Sample List Options** dialogue is **Fields**. This dialogue allows you to add/remove the parameters which appear in the active list, or adjust their position using the up/down buttons. To add a new item click the button; to remove an existing item, click the button. Additionally you can change the existing parameters. To do so, double-click on a parameter and select a new parameter from the combo box. Then press **<Enter>** (on your keyboard) to accept the change, or click on another field in the dialogue.

When you are finished press the **[Close]** button at the bottom of the dialogue to apply the changes to the active list.

The samples / stations displayed in the Active List are sorted in ascending order according to the fields listed in the second tab, **Order by** (as shown below).

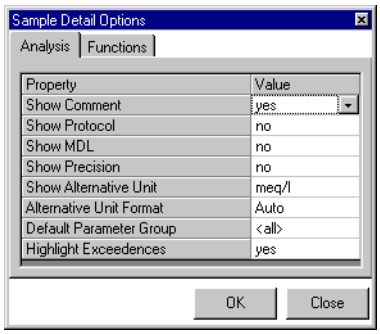


This dialogue allows you to specify the **Sort** options for your active list. The active list will be ordered based on the first (top) field which is defined in this tab. The list will then be further sorted based on the second field in this dialogue, and so forth.

To move fields in this dialogue, use the  or  buttons. To add or remove fields, use the  or  buttons. To change the existing fields, double-click on an existing field, select a new field from the combo box and press **<Enter>** on your keyboard to accept the changes. When you are finished, press the **[Close]** button at the bottom of the dialogue to apply the changes to the active list.

NOTE: The active samples list and the active stations list each has its own sorting options. To access the sorting options for the Active Stations list, ensure the **Stations** tab is selected in the active list when you select **View > Options**.

Options - Sample Details



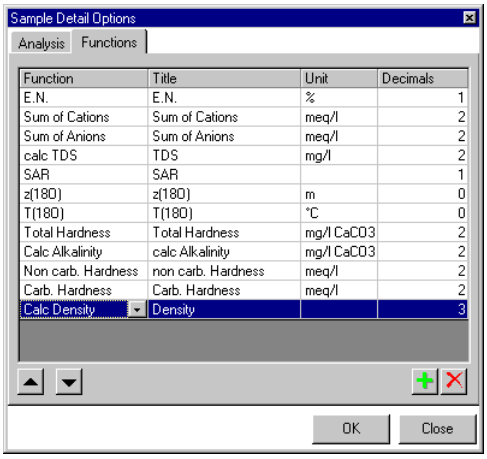
When a **Sample Details** window is active, click **Options** from the **View** menu to access the **Sample Details Options** dialogue as shown on the right.

Under the **Analysis** tab, you can edit the settings of the Sample Details window, specifically the **Measured** parameters tab. Fields can be turned on or off, by selecting  button and **Yes/No** from the combo box. You may also select the alternative units, a default parameter group, and enable/ disable guideline exceedances (to activate or deactivate this option). You may show or hide the following columns:

Comment: allows you to add a comment for each measured value
Protocol: protocol used for sample measurement
MDL: maximum detectable limit
Precision: precision of measurement
Alternative unit: displays an alternate unit (e.g. meq/L when a value is expressed in mg/L)

If one or all of these parameters are not needed, you may hide the respective columns from the Sample Details window.

Under the **Functions** tab (shown on the right) you may edit the settings of the calculations which appear under the **Calculated** tab in the Sample Details window. These options allow you to control the appearance of the Calculated fields. The names of the Calculated parameters can be edited under the **Title** column. The units and number of decimal places for the Calculated values can also be adjusted. The order of the calculated parameters can be arranged using the  and  arrows.



Functions can also be added or removed using the  and  buttons respectively. Once you are finished, press the **[OK]** button to return to the Sample Details window.

For more details on the Calculations performed by AquaChem, please see the **File > Database > Calculations** (section 3.11.8, Calculations).

Options - Table View

If you select **View > Options** while a **Table View** window is open, this will load the **Table View Settings** dialogue for defining the view of the Table (i.e. available parameters, table layout, etc.). Alternatively, you may use the **Options**  icon from the AquaChem toolbar.

Options - Plots

If you select **View > Options** while a **Plot** window is open, this will load the **Plot Options** dialogue for that plot type.

Options - Reports

If you select **Options** from the **View** menu, while a **Report** window is open, this will load the **Report Options** dialogue for that specific Report type.

3.4 Filter Menu

The options under the **Filter** menu allow you to temporarily "hide" samples, and work with only a few samples or a subset of your database. Omitted samples will be excluded from any plots, tables, reports, or calculations. These options allow you to focus on specific sites or locations, and produce site-specific plots and reports.

NOTE: The Filter options apply to both the **Stations** and the **Samples**. For example, when a station is temporarily omitted, all samples associated with that station will also be temporarily omitted from the active list.

Show All

Using this command restores all the samples or stations to your active list, e.g. any samples that you omit can by reinstated into the active list by choosing **Show All** (Ctrl-A) option from the **Filter** menu.

Show only selected

This option allows you to display only the selected sample(s) or station(s). All non-selected records will be hidden from the active list. When selecting samples/stations in the active list with the mouse, remember that AquaChem supports the standard Windows selection functions: press <**Shift**> or <**Ctrl**> to select multiple records.

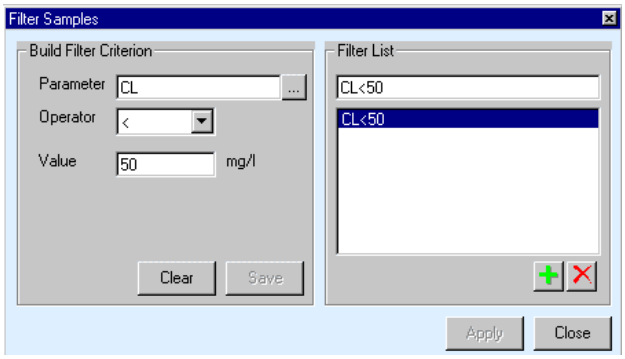
Omit selected

This option hides the selected sample(s) or station(s) from the active list. These samples or stations are not deleted; they are simply not shown in the active list window, so that you may work with a subset of the database.

Custom

When you select **Custom** from the **Filter** menu, you are provided with the options for data filtering. The Custom filter allows you to run a search query and automatically filter out those samples or stations which do not meet the filter criterion.

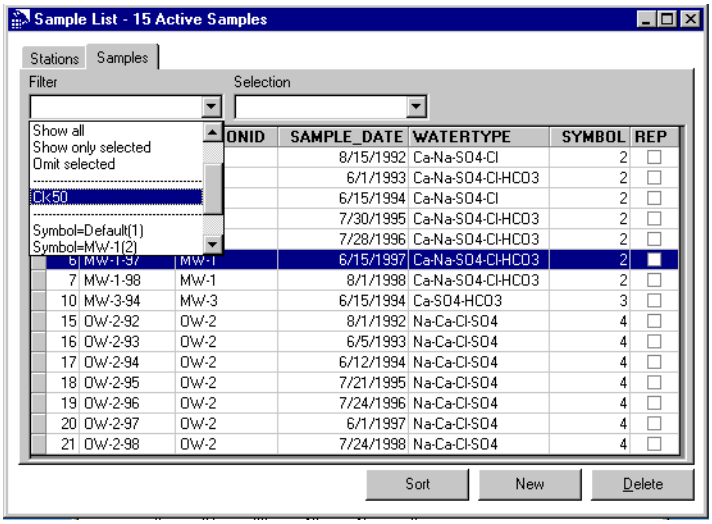
To build and run a custom filter query, select **Custom** from the **Filter** menu and a **Filter Samples** dialogue will appear.



To create a custom Filter:

- Press the button to add a new filter.
- Under the **Filter List** enter a name for this new filter.
- Beside the **Parameter** field, click ... button to access the parameter list and select a **Parameter** from the list.
- Click button and select an **Operator**. You may choose from: <, >, =, LIKE in the combo box.
- Enter a **Value** which corresponds to the operator (ex. Cl < 50 as shown above). The units used for this value correspond to the units used for that parameter, and will be displayed automatically when the parameter is selected.
- Press **[Save]** to save the filter settings.
- Press **[Apply]** and then **[Close]**.

AquaChem will then query the active list for this search criteria. Those samples/stations which do NOT meet the search criterion will be automatically omitted from the active list. To retrieve these samples/stations later, simply press **Filter > Show All**. This query can then be recalled at a later date, by accessing this Filter from the Filter list. In addition, this filter will also show up directly above the active sample/stations list, as shown in the figure below:



Simply choose a filter from the combo box in the upper-left corner, and the filter will be applied to your active samples or stations. You will also note in here, that you may select symbol groups, and filter the active samples list based on the assigned symbols.

NOTE: The filter selection is context sensitive: if the **Samples** tab is active in the main list, the custom filter will allow you to build and run filters on samples; if the **Stations** tab is active, the filter is applied to stations.

Invert Selection

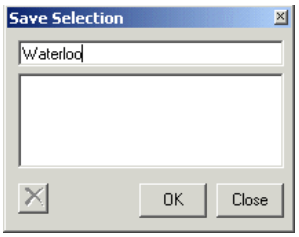
Use this command to select all records that are not selected, and de-select all records that are currently selected.

Select Associated Samples/Stations

Use this command to select all samples which are associated with a station(s) or vice versa. For example, if you are in **Stations** mode and you want to locate all samples which are associated with a selected station, simply click **Filter > Select Associated Samples** then switch to the **Samples** tab and those samples which are associated with that station will be highlighted. This command can be applied to multiple stations or samples. Use the **<Shift>** or **<Ctrl>** keys on your keyboard to select multiple records.

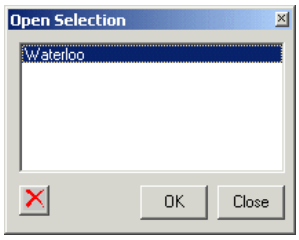
Save Selection

The **Save Selection** command saves the currently selected list of samples or stations to your project database. In the **Save Selection** dialogue enter the name of the file. This file can be opened in later sessions to work with the same subset of the database.



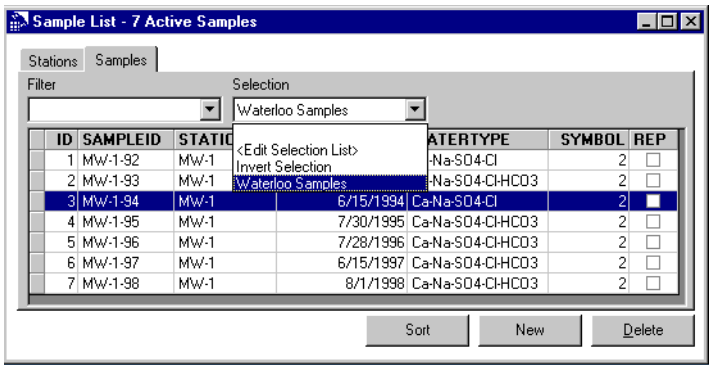
Open Selection

This command allows you to retrieve a previously saved data selection:



In the **Open Selection** dialogue, select a previously saved selection from the list and press **[OK]**. All records belonging to the selection file will then be highlighted in the active list.

If you want to work exclusively with the samples from the selection file, select **Show Only selected** after opening the selection file. Selections can also be retrieved from the active list as shown below:



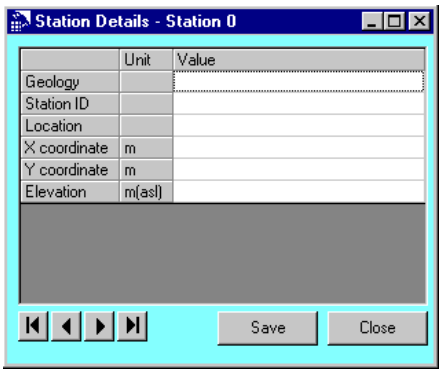
NOTE: Saved selection files can only be opened in the database in which they were created.

3.5 Stations/Samples Menu

The next menu item is **Stations** or **Samples**. This menu is automatically updated to reflect the current mode in AquaChem. If the Samples tab is selected in your list, or if you have a Sample Details window active, then this menu item will show as **Samples**. If the Stations tab is selected in your list, or if you have a Station Details window active, then this menu item will show as **Stations**. Each of the **Stations**/**Samples** menu item is explained below.

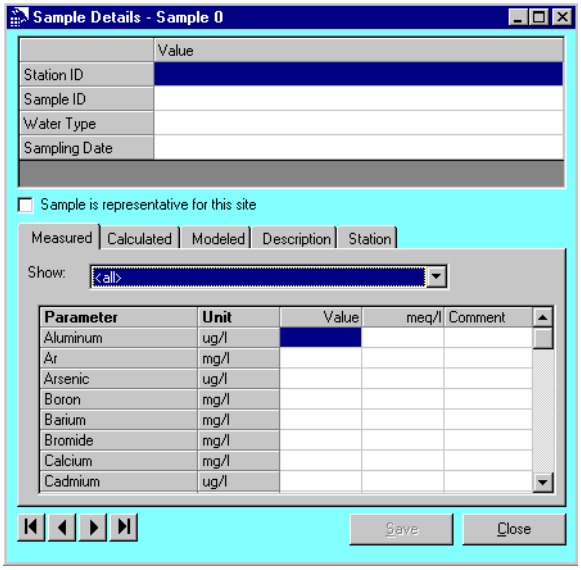
New

This item allows you to create a new sample or a new station. When you select **Stations > New**, you will see the a **Station Details** window:



To add station data, click with your mouse in the input fields and type in the required data. Use the **<Enter>** key to accept the value and advance to the cell below. Click the **[Save]** button at the bottom of the details window to add the new record to your database.

When you select **Samples > New**, you will see a **Sample Details** window:



NOTE: You must have at least one pre-defined station in your database before creating a new sample. Therefore, when you create a new database, you must first create a minimum of one station; then you may create a new sample(s) and **Assign** a station to this new sample(s).

To add sample data, click with your mouse in the input fields and type in the required data. Click the **[Save]** button at the bottom of the details window to add the new record to your database.

NOTE: AquaChem requires you to use a point "**.**" decimal for all numeric data. In addition, ensure that your Computer Settings - Regional Settings are set to English, U.S. to support this format.

Duplicate

Creates a duplicate sample or station. All station parameters are copied over from the currently selected sample or station. Duplicating samples can be an efficient way of creating multiple samples belonging to the same station.

Edit

Opens the details window for the selected sample or station.

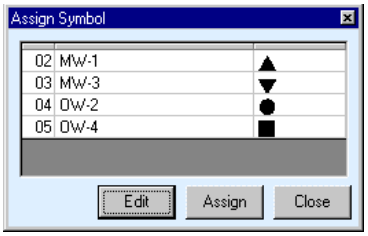
Delete

Deletes the selected sample or station.

Assign Symbol

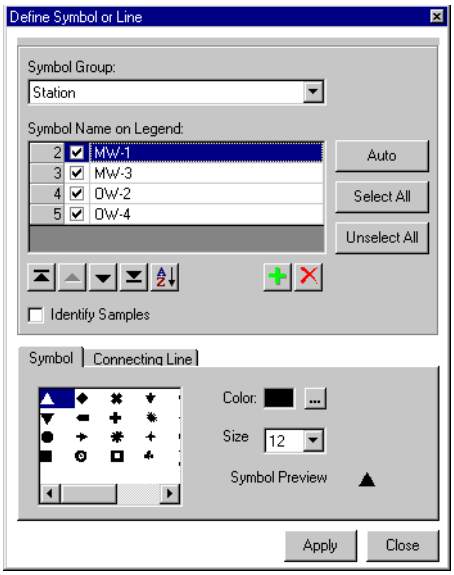
The **Assign Symbol** option allows you to assign symbols to your samples. This option is only available when you are in **Samples** mode.

To assign symbols to samples:



- Select the desired sample(s) in your active list
- From the main menu, select **Samples > Assign Symbol** (or use the **Assign Symbol** icon from the main tool bar).
- The **Assign Symbol** dialogue will appear, and provide a list of the available Symbol names and the corresponding symbols.
- Choose one symbol from this list and click the **[Assign]** button. This symbol will then be assigned to the selected sample(s).
- To return to the active list of samples press **[Close]**.

To edit the symbol options, press the **[Edit]** button. This will load the **Define Symbol or Line** dialogue as shown below.

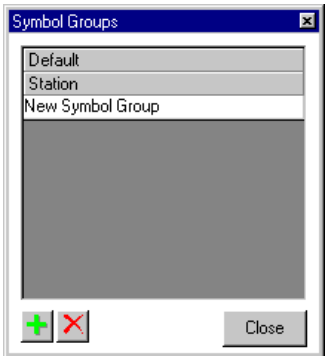


In this dialogue, you can create symbols and symbol groups, and define the symbol characteristics. The upper portion of this dialogue contains the **Symbol Group** and the

symbols belonging to this group. You can create multiple symbol groups for one sample, based on your current project objectives. For example, you may want to assign symbols based on Location, however you may also want to assign symbols based on Geology or another variable. To do this, simply create a new symbol group, define the symbols, and assign these symbols to the samples. However, only one symbol group may be plotted at a time.

There are two default symbol groups included with every Aquachem database: **Default** and **Station**. The Default symbol group includes one symbol, called Default. The Station symbol group includes one symbol for each unique station ID that is created in your database. Each time a new station is created in your database, a corresponding symbol will be created in the Station symbol group; the symbol name will be identical to the Station ID.

To create new symbol groups, choose the **<Edit>** option from the combo box below the **Symbol Group** and the **Symbol Groups** dialogue will appear as shown below



- Click  button to create a new symbol group and then enter a name for the new symbol group
- Click  button to delete existing symbol groups
- Click **[Close]** to return to the previous dialogue

The **Symbol Name on Legend** frame lists the available symbols, their name and status, for the corresponding symbol group.

To add or remove symbols from a symbol group:

- Click  button to add a symbol to the group
- Click on the delete button  delete the selected symbol

The symbols with a check mark beside them are active; as a result, the samples associated with these symbols will be displayed on the open plots. To remove a group of sample data points from all of the open graphs, simply click on the appropriate check box to de-activate the corresponding symbols. The following buttons also appear in this dialogue:

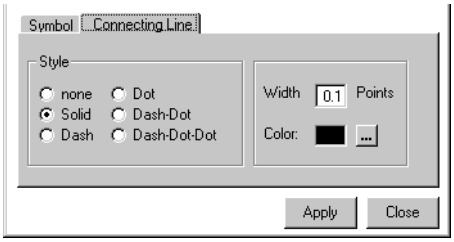
To activate all symbols, press the **[Select All]** button.

To deactivate all symbols, press the **[Unselect All]** button. To move symbols in this list, use the up/down arrow buttons.

To sort the symbols alphabetically.

The **Identify Samples** option is used to highlight the samples in the active list that are associated with the selected symbol.

The lower section of this dialogue allows you to define the shape and color of the symbols and lines that appear in the AquaChem plots. Under the **Symbol** tab you will see different shapes of the symbols. The **Color** and **Size** of the symbol can be modified and **Symbol Previewed** as it will appear on the plots. AquaChem now uses “True type fonts” for symbols on plots and graphs. As such, there is an unlimited number of symbols that you can use for your database.

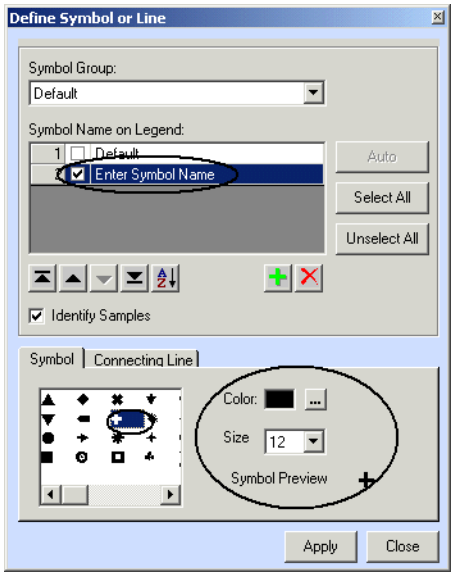


Under the **Connecting Line** tab you can select **Style**, **Width** and **Color**. Each symbol is associated with a particular line style. This line style, the width of the line, and the line color can be customized for each symbol. The **Style** field displays a selection of six line styles, a line width, and a line color that can be displayed in the Depth Profile Plot, Schoeller graph and the Time Series graph to connect associated data points.

Click **[Apply]** to save changes you made to the symbols. To return to the main AquaChem window, press the **[Close]** button.

Creating New Symbols

Follow the instructions below to create a new symbol:



- Select a **Symbol Group** from the combo box at the top of this dialogue
- Press the button and a new field will be added to the list of symbols
- Enter a name for the new symbol
- Then press the **<Enter>** key (on your keyboard) to accept the new name
- Define the symbol properties in the bottom section of this dialogue
- Choose a symbol character from the list of available symbols
- Choose a **Color** for the new symbol. To access the color options, press the ... button beside the color field, and select a color from the Color palette.
- Choose a **Size** for the symbol. A list of font sizes can be accessed by clicking the button from the combo box.
- Press **[Apply]** to create the symbol
- Press **[Close]** and return to your sample list

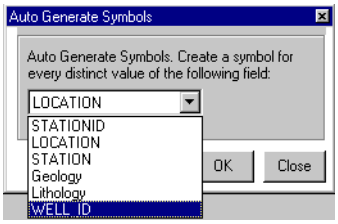
Now use the **Samples > Assign Symbol** option to assign this symbol to the desired samples. If done successfully, the active samples window will display a column listing the symbol number which is assigned to each sample.

Auto Generate Symbols

AquaChem v.4.0 includes a convenient feature that allows you to automatically create symbols based on station database parameters. Press the **[Auto]** button in the **Define Symbol or Line** dialogue to load this option.

> **NOTE**: The auto generate symbols option is not available for the Default symbol group. You must first create a new symbol group in order to activate the **[Auto]** button and to use this option.

In the **Auto Generate Symbols** dialogue, you will be prompted to choose a parameter for which symbols will be automatically generated. The available parameters are **Station Description Parameters** as defined in your database template. For example, if you choose **Location** as the field there will be a symbol generated for each unique Location in your database.



A unique symbol character will be generated for each symbol group, and will use the default font size of 12 and default color black.

Select the desired field and click **[OK]** to return to the **Define Symbol or Line** dialogue, where you will see the new symbols which were automatically generated. You now have the option of modifying these new symbols (i.e. the shape, color, name, size, etc.).

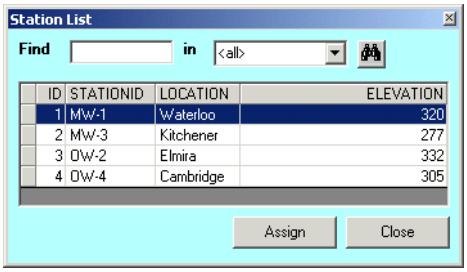
The new symbols are automatically assigned to the samples in your database; the symbols will be assigned to the matching parameter for that sample. For example, if you automatically generate five symbol groups based on Location, AquaChem will search your database for all instances of the Location parameter, and create a symbol for each unique entry for Location.

Each symbol will have a symbol name that corresponds to the different available Locations in your database. After the symbols are created, AquaChem will assign the proper symbol to each sample which contains that specific Location entry. (e.g. symbol name = Baden, then this symbol will be assigned to ALL samples which have a station Location = Baden).

Assign Station

The **Assign Station** option allows you to assign a station to the selected sample. This menu item is only available when a **Sample Details** window is active.

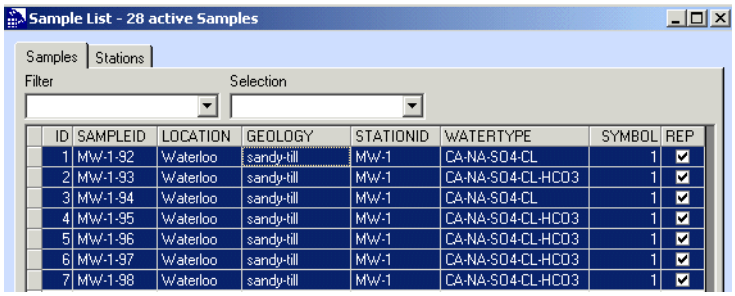
When you select **Samples > Assign Station** from the main menu, a **Station List** dialogue (as shown here) will appear with a list of the available stations in your database.



From this dialogue, you may select a station directly from the list; or if you have large list of stations, the **Find** feature at the top of this window can be helpful. Once you have located the desired station for this sample, press the **[Assign]** button at the bottom of this dialogue and this will return you to the Sample Details window.

Representative On / Off

This option defines the **Representative** samples flag for the selected sample(s). A representative sample is indicated by the presence of a check mark in the **Active Samples** window as shown below.



ID	SAMPLEID	LOCATION	GEOLOGY	STATIONID	WATERTYPE	SYMBOL	REP
1	MW-1-92	Waterloo	sandy-till	MW-1	CA-NA-SO4-CL	1	☑
2	MW-1-93	Waterloo	sandy-till	MW-1	CA-NA-SO4-CL-HCO3	1	☑
3	MW-1-94	Waterloo	sandy-till	MW-1	CA-NA-SO4-CL	1	☑
4	MW-1-95	Waterloo	sandy-till	MW-1	CA-NA-SO4-CL-HCO3	1	☑
5	MW-1-96	Waterloo	sandy-till	MW-1	CA-NA-SO4-CL-HCO3	1	☑
6	MW-1-97	Waterloo	sandy-till	MW-1	CA-NA-SO4-CL-HCO3	1	☑
7	MW-1-98	Waterloo	sandy-till	MW-1	CA-NA-SO4-CL-HCO3	1	☑

When you perform a search or calculation, you may choose to use only samples in the active list which are representative of each site.

NOTE: The Representative menu item is only available when you are in the samples mode.

- To enable this option, choose **Sample > Representative > On.**
- To disable this option, select **Sample > Representative > Off** (or manually remove the check mark in the Sample Details window).

3.6 Plots Menu

The following section provides a brief summary of the commands in the **Plots** menu. For more details on the AquaChem plots and the plot options, please refer to Chapter 4.

New

This item allows you to create a new plot.

Open Configuration

Opens a previously saved plot configuration.

Save Configuration

Saves the current set of plots and their settings to the current AquaChem database.

Save Plot Data

This command opens a worksheet containing the plot data of the current plot. This feature is useful if you want to use another plotting program. This menu item is only active when a plot window is loaded.

To save the data choose **Save** from the **File** menu and the data can be saved as .TXT or .CSV format.

Close All Plots

Closes all plot windows.

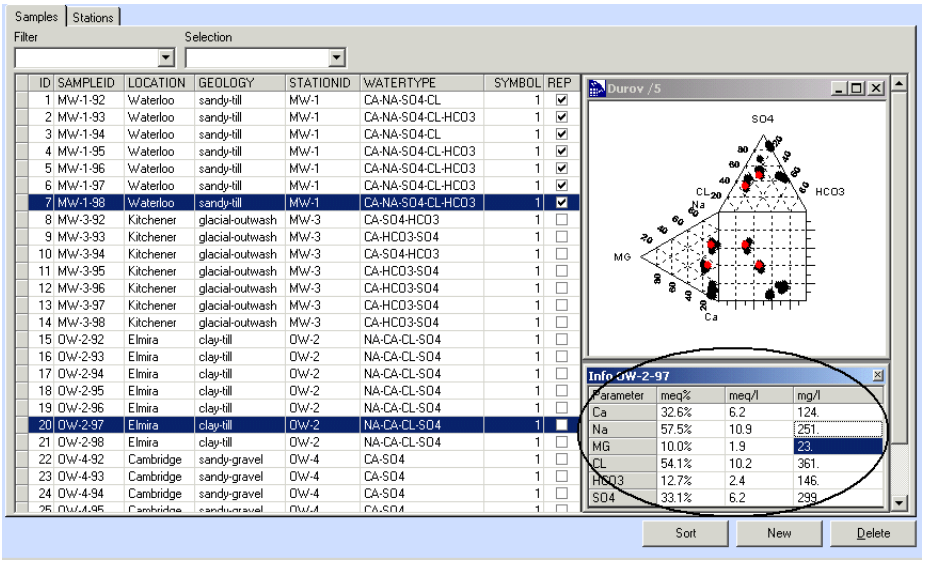
Define Symbol or Line

Loads the **Define Symbol or Line** dialogue for defining symbol and line properties as they appear in the plots and graphs. For more details on this dialogue, please refer to the sections Assign Symbol, Creating New Symbols**,** and Auto Generate Symbols above.

Show Sample Data

If this option is selected, AquaChem will display a small dialogue with the data for the selected sample. Simply click on a sample point from the plot and the **Info** data dialogue will appear. Each time you click on a new sample point, the new data is loaded into dialogue. An example is shown below:

NOTE: You may need to re-arrange the positions of your windows in order to see the sample data dialogue.



Identify Plot Data

The Identify option allows you to link the plotted data to the samples in the active list. This allows you to click on a point in the graph and view the corresponding sample in the active list. This is useful when you have a large number of samples plotted on one plot, and you want to identify outliers.

There are three options available for selecting and identifying points on a plot: **None**, **Selected Plot**, and **All Plots**. The default mode to identify points is on All Plots; this means that all data points on all plots are linked to the database. These three options are described below:

None

If you click on a plot, no samples will be highlighted. The data points on the graphs are not linked to the database which means that samples are not identified. When you have several open graphs and a large database with many samples, it may be convenient to have no link between the graphs and the database in order to increase the speed of the various AquaChem operations.

Selected Plot

Only the data points in the active graph are linked to the database. The plotted point is activated (turns red) and is selected in the sample list. This mode is useful if you are working with a large data set and want to focus on just one graph.

All plots

The sampling point of the corresponding sample is activated on all plot windows and on the sample list. If you are working with several graphs, you can identify a sample in all plots as well as in the sample list by clicking near a point in any of the plots, or by clicking on a sample in the active list. The sample will become selected in the active list, and the corresponding data points will be highlighted in red in all the open plot windows.

3.7 Reports Menu

The **Reports** allow you to create a summary of your data from your AquaChem database. AquaChem generates seven pre-defined reports and also allows you to create your own report templates.

These reports are all generated in a separate Report window in a spreadsheet view. The reports can be printed 'as is' using the **[Print]** button on the lower-left corner of the window or the information can be easily saved using the **[Save]** command.

The following is a brief summary of the options under the **Reports** menu. For more details on Reports, please refer to Chapter 5.

Compare Samples

The **Compare Samples** report allows you to compare a sample in your database to another sample or multiple samples. The Compare Samples report uses a linear regression algorithm to generate the **Correlation coefficient** and the **Euclidean distance** between a selected sample and all other active samples. Samples having a chemical composition similar to the selected sample will have a correlation close to 1.

Correlation Matrix

The **Correlation Matrix** report generates a correlation matrix for a specified number of sample parameters that are common to all active samples. A linear regression routine calculates the regression coefficient (r), and the slope and intercept of the regression line.

Mix Samples

The **Mix Samples** report generates solution concentrations resulting from the step-wise mixing of specified proportions of two selected samples from the project database.

Water Quality Standards

The **Water Quality Standards** report provides a summary of parameters exceeding the established Water Quality Standards for the selected sample. The selected samples are compared to the pre-defined Water Quality Standards as specified in the **Preferences** in the **File** menu.

Reliability Check

The **Reliability Check** report allows you to confirm the validity of the measured sample data. There are a number of tests provided in AquaChem which can provide insight into the reliability of your analysis.

Rock Source Deduction

This report allows you to determine the possible origin of the water analysis. The results are a general overview, based on ions ratios found in the selected sample. If results do not meet expectations the result should be confirmed with more detailed study, based on multiple samples, aquifer mineralogy analysis, modeling, and plots.

Statistics

The **Statistics** report shows the general statistics for all visible or selected samples.

Sample Summary

The **Sample Summary** report provides a general overview of a sample including major ions, hydrochemical facies (e.g. Na-Cl), calculated hardness, ion balance, ion ratios, etc.

GeoThermometers

This reports displays some commonly used GeoThermometers.

Isotopes

This report displays values for common isotopes.

Report Designer

The **Report Designer** allows you to customize your own reports based on a single sample. The user defined reports may contain any parameter, ratio of parameters or function values. It is also possible to add a template and create a print ready output for your report.

3.8 Tools Menu

The **Tools** menu provides access to the data analysis tools, including converters, calculators, LookUp Tables, and access to the PHREEQC modeling interface. The following is a brief summary of the options under the **Tools** menu. For more details on Tools, please refer to Tools (Chapter 6).

Calculators

When you access the **Calculator** option from the Tools menu, you will find the following options:

Aquachem Function

The **Aquachem Function** is a complement to the Calculated parameters tab available in the Sample Details window. It allows you to calculate any function in any available unit quickly and easily, based on the selected sample. The calculations in the Sample Details window are fixed and typically contain the most commonly used calculations. However, if you want to use some of the other calculations the **Aquachem Function** dialogue provides these options.

Decay Calculator

This tool allows you to calculate the degradation of a species.

You may choose to calculate:

- **Concentration after a specified amount of time**; or you may determine the
- **Time to reach a specified concentration**.

AquaChem includes half-life's for more than 300 species, for physical phases including air, soil, groundwater and surface water. These half-life's are taken from the following reference.

Ph. Howard et al. (1991): Handbook of Environmental Degradation Rates.

Find Missing Major Ion

This tool helps you to fill in missing data for missing cations or anions, using the charge balance and existing measured values for other ions for the sample.

Formula Weight Calculator

This tool helps you to calculate the formula weight based on a user-defined formula.

Volume Concentration Converter

This converter is used for samples with measured organic chemicals. It allows you to convert measured concentrations in ppm by volume (ppmV), to mg/m3 at a specified temperature.

Special Conversions

This tool provides conversions for non-linear geochemical calculations.

Species Converter

This tool allows you to convert any species into a different form. This is useful to express a measured amount of a parameter as a different aqueous species when expressed in mg/L.

Unit Calculator

This tool performs basic unit conversions for length, time, volume, density, mass, etc.

Look Up Tables

The **Look up Tables** shows the tables that are defined in the **File > Database > LookUp Tables** dialogue. These tables allow you to quickly find information for use in AquaChem.

Degradation Rates

This look up table provides a list of degradation rates for common organic chemicals.

PHREEQC Phases

This look up table provides a list of commonly used minerals including formula and formula weights.

Periodic Table

This table provides information for the elements of the periodic table.

Adsorption Isotherms

Provides information for adsorption parameters for common organic chemicals.

Modeling

AquaChem has a built-in link to the PHREEQC geochemical modeling program, that is capable of creating one or more solutions from the water quality samples in your AquaChem database. The **Modeling** option under the **Tools** menu provides links to the various options for PHREEQC. The following is a brief introduction to the modeling features included with AquaChem. For more details, please see Chapter 6 and 7.

Calculate Saturation Indices and Activities

This command will run PHREEQC for the samples selected in your active list. PHREEQC will calculate saturation indices and activities for those parameters which are defined in your database (those parameters listed in the Modeled Parameters tab). The results will automatically be saved back to the Sample Details table, for the selected samples.

Calculate pH

This allows you to calculate the pH for the selected sample. The simulation is based on the assumption that the solution is in equilibrium with a carbonate mineral. This utility may be used to estimate the pH, in the case where a measured pH value does not exist. However, this is calculated based on the assumption that the groundwater sample in question, flows in a carbonate aquifer. Alternatively, if a measured pH value exists, you can use this tool to calculate pH, and make comparisons.

Calculate Eh

This allows you to calculate the Eh for the selected sample. The Eh is calculated based on the redox speciation, using the Nernst Equation. Each Redox couple gives an individual Eh value which in cases of equilibrium conditions, should be reasonable. This menu item launches PHREEQC to search for available redox couples and to calculate pe and Eh values for each couple.

PHREEQC (Basic)

This will allow you to create an input file for PHREEQC, and run a simplified version of PHREEQC. The more advanced features (Inverse Modeling, Kinetics, and Advection/Transport) are not included in this option. To utilize these features, you may load one of the USGS's full versions of PHREEQC as explained below.

PHREEQC (Advanced)

This will load an external window, containing one of the USGS's PHREEQC interfaces (PHREEQC-Interactive or PHREEQC for Windows). This will allow you to use the full

features of the PHREEQC modeling program, using your AquaChem samples as initial solutions.

3.9 Window Menu

All open AquaChem windows are listed in the Windows drop down menu, and can be activated by clicking the window's title in the Windows drop down menu.

Tile Vertical

Arranges open windows side by side.

Tile Horizontal

Arranges open windows one above the other.

Cascade

Cascades open windows.

Arrange Icons

Organizes icons of minimized windows along the bottom of the parent window.

3.10 Help Menu

Contents

Displays the AquaChem On-line Help.

Index

Displays the Help index.

About

Displays the AquaChem version number and information on how to contact Waterloo Hydrogeologic, Inc.

This concludes a review of the AquaChem menu items. The following sections describes the components of an AquaChem database.

3.11 The AquaChem Database

In this section, you will find information on the AquaChem database. This includes:

- Parameters
- Parameter Groups
- Aliases
- Lookup Tables
- Water Quality Standards
- Ranges
- Thermometers, and
- Calculations

An AquaChem project database files are saved in a Microsoft Access 2000 relational database format. The projects are saved with a unique file extension (filename.**AQC**). This is done for two reasons:

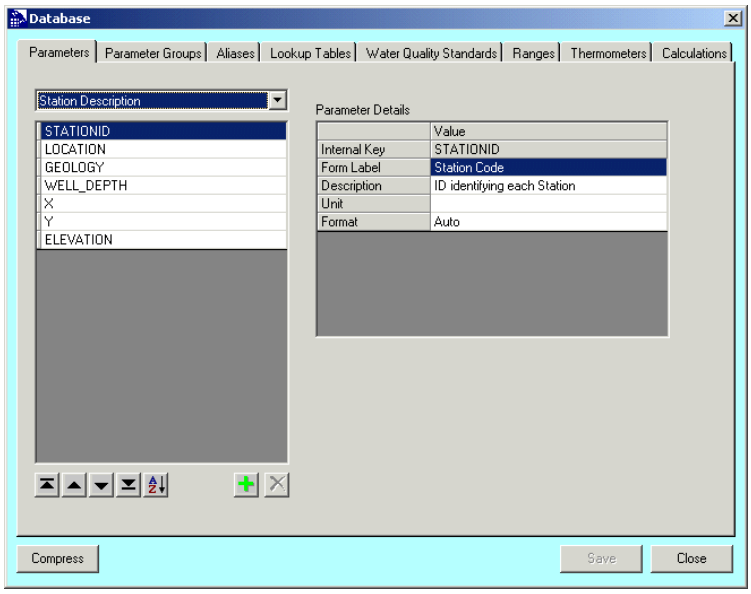
1. This prevents any confusion or possible corruption of the file if it were to be accidentally opened in Access, and critical changes were made to the data structure or even to the data itself; and
2. This ensures that only AquaChem projects are opened in AquaChem, and that non-supported files are not opened resulting in possible corruption or data loss.

However, it is still possible to view/edit an AquaChem database file using MS Access. Simply launch MSAccess and open this database file, using the **File > Open** command. It is recommended that you first make a back-up of your database file, before modifying it in MSAccess.

Each AquaChem database relies upon a central database, the Aquachem.MDB database file. This file is a central database that holds information that is common to all databases (e.g. code tables, a set of parameters that can be used to define parameters in a project database, template layouts, etc.). This file is automatically copied to your AquaChem40 installation folder; the file location and contents should not be modified.

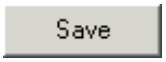
An AquaChem database may contain an unlimited number of samples, depending on the number of parameters it uses and the amount of memory available on your PC. Working with too many samples can slow some operations even though you are only working with a portion of the database. Therefore, working with several databases containing less than 5,000 samples may be more efficient than using one large database.

To view and modify the AquaChem database structure, select **File > Database** from the main menu while the Samples/Stations list is active. The following dialogue should appear:



The **Database** dialogue contains numerous options for modifying parameters and database settings for your AquaChem database.

At the bottom of the Database dialogue, you will see three buttons:



The **Save** button will save any changes you make to your database.

The **Close** button will close the Database options dialogue, and return you to the main AquaChem window.

The **Compress** button will compress your database. Your project database file size may become large if you have a large number of samples, and are continuously deleting samples. Compressing the database will compact and repair your database, and may make the file size more manageable. AquaChem will create a backup copy of the uncompressed database file, with the file extension .SAV. Should you encounter problems with the new compressed file, simply delete this, and restore the previous file by renaming the .SAV file with the extension .AQC.

The **Database** dialogue contains several tabs. Each tab controls the internal options for the database which include:

- Parameters

- Parameter Groups
- Aliases
- Lookup Tables
- Water Quality Standards
- Ranges
- Thermometers, and
- Calculations

3.11.1 Parameters

The **Parameters** tab allows you to modify the data structure of the current AquaChem database project by adding or deleting parameter fields from each of the four parameter categories. The **Parameters** tab can also be used to modify the attributes of each parameter (e.g. Display label, Internal name, Molecular weight, Charge, Units, etc.) or to change to order in which the parameters are displayed in the Sample Details window.

In an AquaChem database there are four categories of parameters:

- **Station Description Parameters**
- **Sample Description Parameters**
- **Measured Parameters,** and
- **Modeled Parameters**

A detailed description of each parameter category follows below:

Station Description Parameters

These are parameters which contain general information about the station. This data is entered once for every individual station. The station can then be assigned to a single sample or multiple samples. Typical parameters for the stations are: station name, ID, location, area, X,Y coordinates, elevation, and well depth. Station Description parameter values can be text or numbers. An AquaChem database may contain a maximum of 255 Station Description parameters.

Sample Description Parameters

These are parameters which contain general information about the sample. This category typically includes alphanumeric or data types such as sample ID, geology, sampling date, etc. Sample Description parameter values can be text or numbers. An AquaChem database may contain a maximum of 255 Sample Description parameters.

Measured Parameters

These are parameters that are either measured at a sampling location (in the field) or derived from a laboratory analysis of a water sample taken from that location. These parameters will contain numerical values for your sample (ex. concentrations for

cations, anions, organic contaminants, pH, TDS, etc.). For these parameters, you may enter a comment for every analyzed value as well as an acceptable Range. An AquaChem database may contain a maximum of 255 Measured parameters.

Modeled Parameters

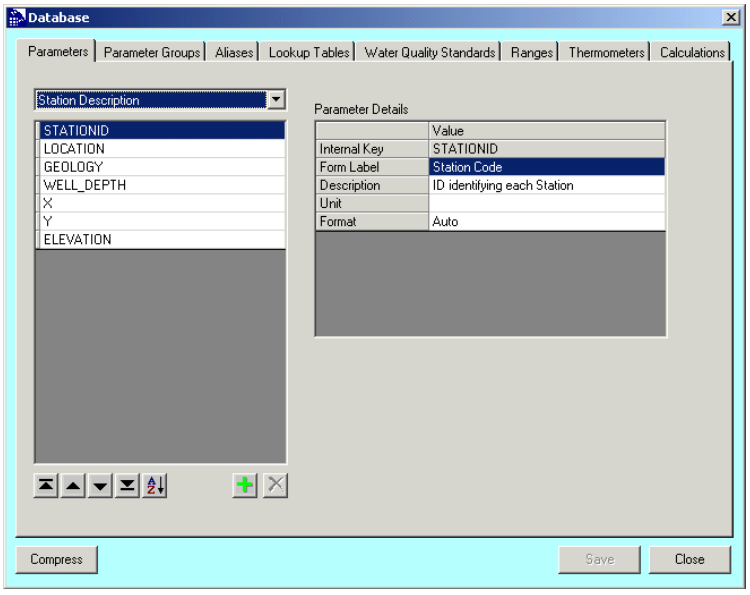
AquaChem provides an integrated graphical interface for geochemical modeling using PHREEQC where the data for each sample in the database can be used as input data for the PHREEQC simulations. Modeled Parameter values are calculated by PHREEQC during a simulation. These parameters can be added to your database template, however the values for each parameter can only be added following a PHREEQC simulation. An AquaChem database may contain a maximum of 255 Modeled parameters.

The Modeled Parameters are very similar to numerical parameters, however you may not add comments, description, or define Ranges. Modeled Parameters appear in a separate tab in the Sample Details window.

For more details on the Modeled Parameters and PHREEQC modeling, please refer to Chapter 6, and “GeoChemical Modeling with PHREEQC (Basic)” (Chapter 7).

Parameter Details

For each Parameter category, you will see a list of parameters belonging to that category appearing on the left side; on the right side, you will see the description and details for each parameter, as shown below:



At the bottom of the Parameters list, you will see several buttons. The function of each button (in order from left to right) is as follows:

Move to top: moves a parameter to the top of the list

Move up: move the parameter up

Move down: move the parameter down

Move to bottom: move the parameter to the bottom of the list

Sort alphabetically: sorts parameter list alphabetically

Add new parameter: adds a new parameter

Delete parameter: deletes the selected parameter(s)

Each parameter has a corresponding name, label, and info, so that it can be easily identified in the database, and incorporated in to plots, calculations, and modelling with PHREEQC. Below is a list of the required fields for the various parameter types.

Sample Description Parameters and **Station Description Parameters** require the following **Parameter Details**:

- Internal Key
- Form Label
- Description
- Unit
- Format

A **Measured Parameter** requires the following **Parameter Details**:

- Internal Key
- Form Label
- Description
- Formula
- Formula Weight (g/Mol)
- Valence
- CAS Registry Number
- Unit
- Format

A **Modeled Parameter** requires the following **Parameter Details**:

- Internal Key
- Form Label
- Description
- Formula
- Formula Weight (g/Mol)
- Valence
- Unit
- Format

NOTE: It is not necessary to have values entered for each field for each parameter. However for reports and plots, it is recommended that you enter as much information as possible.

The following is a brief summary of each of these **Parameter Details**:

Internal Key	This is the internal name defined when the parameter is first created; once a parameter has been created, the internal key cannot be changed.
Form Label	Display label assigned to the parameter so that it can be distinguished in the Sample/Station Details window, and other AquaChem windows and dialogues.
Description	Brief description of the parameter. This information is entered only in this location, and is designed to provide the user with a quick reference. (This field may remain blank if desired).
Formula	Chemical formula for the parameter.
Formula Weight	Formula weight for the measured parameter. For many Measured Parameters, there is an option to calculate the formula weight (select a measured parameter then you will see a **Calculate FMW** button appearing below this dialogue. Press this button and AquaChem will automatically calculate the weight of the parameter, provided the formula is entered and available in the database).
Valence	Positive or negative charge (if applicable).
CAS Registry Number	For measured parameters, if you know the CAS (Chemical Abstracts Service) Registry number, you can enter it in this field. Otherwise, you may leave this field blank.
Unit	Allows you to select the units that will be applied for the selected parameter (mg/L, meq/L, etc.). For all other parameters without a

formula, an editable list of units is displayed. To access this list, simply click in the field beside Unit and press the button to load the list of available units.

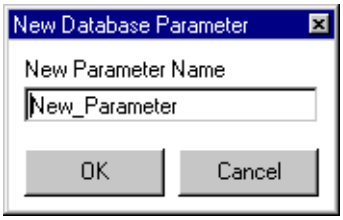
Format Displays the format for a numerical parameter. This field determines how many decimal places will appear for a numerical parameter. To change the display format, simply click in the field beside Format and press the ... button to load the **Format** options dialogue. You can then increase/decrease the number of **Decimal** places using the up/down buttons or select the **Auto** or **Scientific** format for the parameter.

Note that the numeric fields must use a point "**.**" decimal and not a comma "**,**" decimal. The numeric parameter fields do not accept text values such as "ND" or "NA" and will return a value of zero for any text entry. However, AquaChem does accept "greater than" and "less than" values (e.g. <0.01). In addition, AquaChem allows you to recognize or ignore the "greater than" and "less than" values on graphs (see the **File > Preference > Plots** section, and edit the **Approximate Values [</>]** options).

The next section will describe how to add new parameters to your database, and create new parameters.

Adding/Creating New Parameters

If you are adding a **Station Description** or **Sample Description** parameter to your database, follow the steps below:

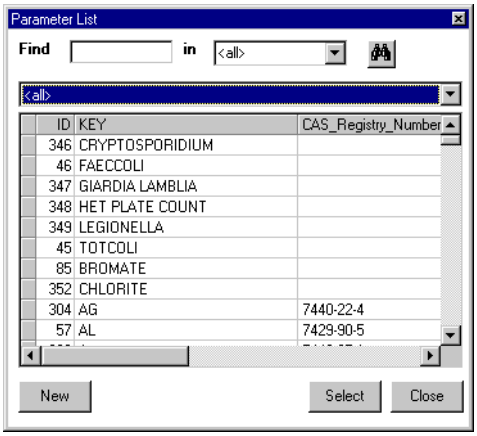


- Select **File > Database** from the main menu (if you have not already done so) and go to the **Parameters** tab.
- Select the **Station Description** or **Sample Description** parameter category from the combo box in the upper left corner of the dialogue.
- Press the button and a **New Database Parameter** dialogue will appear (as shown on the right-hand side).
- In this dialogue type in the name of your new parameter. This name will be used as the Internal Key, Form Label, and Description for the parameter.
- Click **[OK]** and this will return you to the list of parameters.
- Proceed to fill in the required **Parameter Details** for this parameter.

If you are adding a **Measured Parameter**, then follow the steps below:

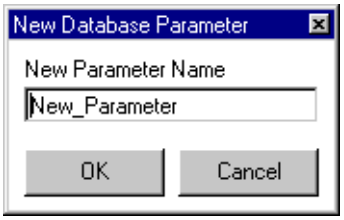
- Select the **Measured Parameters** category from the combo box in the upper left corner of the dialogue.

- Press the button and you will see a **Parameter List** dialogue (as shown on the right-hand side).
- Choose a parameter from the list of available parameters; to add multiple parameters, press the **<Ctrl>** key (on your keyboard) while you select multiple parameters from the source list. You may use the **Find** option to run a query for a parameter name to see if it is available in the AquaChem chemical database. Use the combo box above the parameters list to choose from the various measured parameter categories available in AquaChem (Inorganic, Organic, VOC's, etc.).
- Press the **[Select]** button and the parameter(s) will be added to your database.



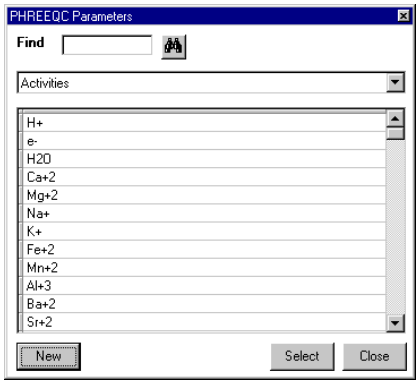
If the parameter that you want to add is **NOT** available in this list, then:

- Click the **[New]** button (in the lower-left corner of the dialogue) and a **New Database Parameter** dialogue (as shown to the right) will appear.
- Type in the name of your new parameter; this may be a formula or full chemical name. This name will be used as the Internal Key, Form Label, and Description for the new parameter.
- Click **[OK]** and you will return to the **Database** options dialogue.
- Proceed to fill in the required **Parameter Details** for this parameter.



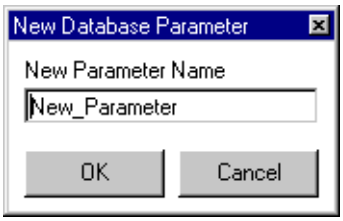
If you are adding a **Modeled Parameter**, follow the steps below:

- Select the **Modeled Parameters** category from the combo box in the upper-left corner of the dialogue.
- Press the button and you will see a **PHREEQC Parameters** dialogue (as shown on the right-hand side).
- Choose a parameter from the list of available parameters. To add multiple parameters, press the <Ctrl> key (on your keyboard) while you select multiple parameters from the source list. You may use the **Find** option to run a query for a parameter name to see if it is available in the AquaChem chemical database. Use the combo box at the top of this dialogue to choose from the various parameter categories available in AquaChem (**Activities**, **Saturation Indices**).



- Press the **[Select]** button and the parameter(s) will be added to your template.

If the parameter that you want to add is **NOT** available in this list, then:



- Click the **[New]** button (in the lower-left corner of the dialogue) and a **New Database Parameter** dialogue (as shown to the right) will appear.
- Type in the name of your new parameter. It is important that the name for new modeled parameter matches the names used in the PHREEQC thermodynamic database for phases (minerals) or species. When selected from the list, this will ensure that the names are matched successfully. This name will be used as the Internal Key, Form Label, and Description for the new parameter.
- Click **[OK]** and you will return to the **Database** options dialogue.
- Proceed to fill in the required **Parameter Details** for this parameter.

NOTE: Parameter names should contain numbers and letters only; do not use any other characters, and/or spaces in the parameter names.

Upon returning to the Parameter list, you must then enter the remaining required parameter details including the description, units, formula, format etc. All measured chemical parameters should have a formula weight specified. If you do not know the molecular weight of a chemical parameter, press the **Calculate FMW** button below the parameter details and AquaChem will read the formula from the field and insert an appropriate molecular weight according to the Periodic Table of Elements. You may also use the Formula Weight Calculator tool, to determine the FMW. Cations and Anions must be accompanied by their **Valence** (which can be a positive or negative number).

The Format field is set to **Auto** by default. To choose a new display format for a parameter, click once in the **Format** field, and then press the ... button and you will see the dialogue as shown on the right-hand side.

The **Format** options allow you to specify the number of **Decimal** places for measured parameters, and specify if the value will be in **Scientific** or whole number format. If **Auto** is selected, then AquaChem will determine the optimal number of decimal places for that parameter. This may result in a "hiding" of a 0 after a decimal place (for example, 7.10 may be displayed as 7.1). To correct this, disable the Auto option, and increase the number of decimals to the desired amount. Once you are finished, press **[OK]** to accept changes or **[Close]** to return to the previous dialogue.

Deleting Parameters

To remove a parameter from your database, simply select the parameter from the parameters list on the left side of the dialogue and click the  button. To delete several parameters press the <Ctrl> key on your keyboard while you select multiple parameters from the source list, then press  button.

Mandatory Parameters

AquaChem has several parameters which are required for EVERY database, and therefore cannot be deleted from the database. These parameters are needed by various plots, reports, and calculations. If a mandatory parameter is selected, the delete button becomes disabled.

The following is a list of mandatory parameters for an AquaChem database.

Mandatory Sample Description Parameters:

Comment

Sample_Date

SampleID

WaterType

Mandatory Station Description Parameters:

StationID

Location

Elevation

X

Y

Mandatory Measured Parameters:

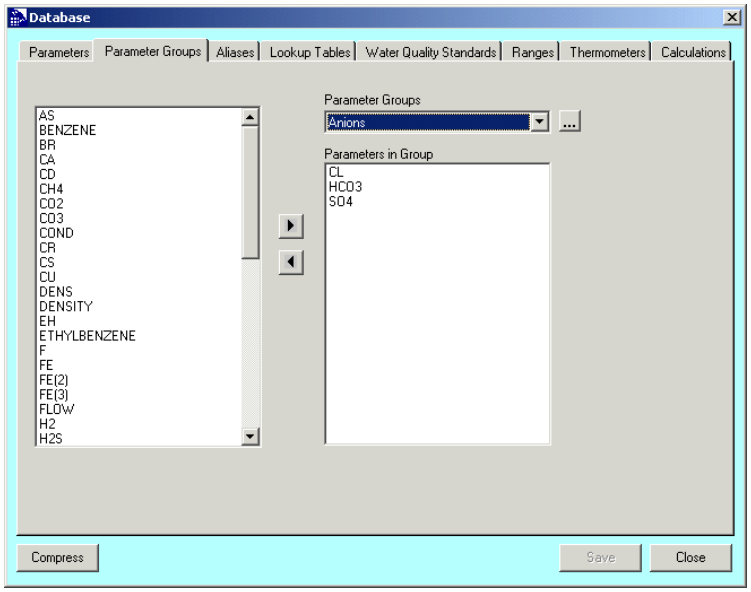
Once you have made changes to the Parameters in your database structure, press **[Save]** to accept these changes.

Ca	HCO3	SAMPLE_DEPTH
Cl	K	Si
CO3	Mg	SO4
COND	Na	TDS

DENSITY	pH	TEMP
Eh		

3.11.2 Parameter Groups

The second tab in the **Database** dialogue is the **Parameter Groups** tab (as shown below):



The **Parameter Groups** options allow you to sort measured numerical parameters into groups, providing a quick and easy view of specific sample data. These parameter groups are created in this dialogue, and then are accessible in the Sample Details window.

For your convenience, AquaChem comes with the following pre-defined parameter groups.

- Hide Non-Detects (hides all parameters for which there are no assigned measurement values)
- Anions (e.g. Cl^-, F^-, SO_4^{2-} etc.)
- Cations (e.g. Ca^{2+}, Na^+, K^+, Mg^{2+}, etc.),
- Gas (O2, CO2, NO2, etc.)
- Isotopes (18O, 2H, 14C, etc.)
- Organic Chemicals (BTEX, Vinyl Chloride, etc.)
- Overview

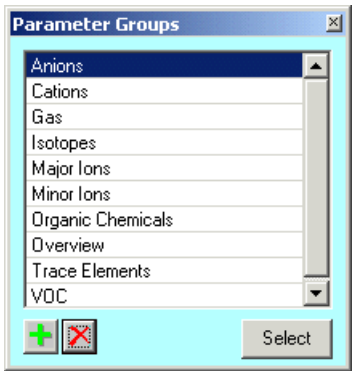
By selecting a parameter group from the combo box, you can view which parameters belong in a selected group; one parameter may belong to multiple parameter groups. To add/remove parameters from a parameter group, simply select the parameter from either the full list on the left side, or the group list on the right side, and press the ▶ or ◀ button to move the parameters accordingly.

You may also create new parameter groups, and add any combination of measured parameters to this new group. This is explained below.

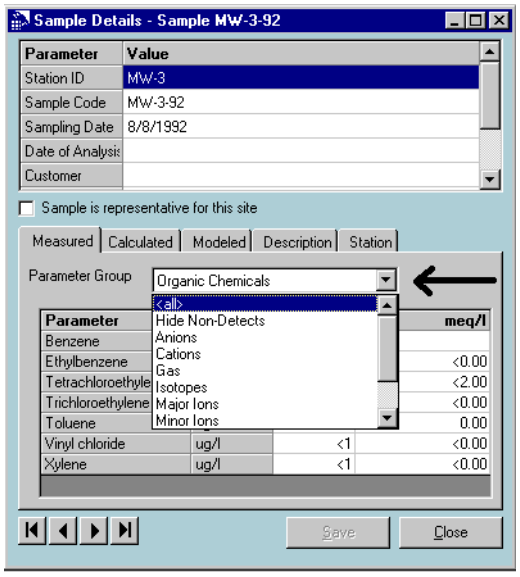
Creating New Parameter Groups

To create a new parameter group:

- Press the ... button beside the list of **Parameter Groups**:
- In the **Parameter Groups** dialogue that appears, press the + button to add a new item.
- Double click on this label and type in a name for this new group. (To delete existing parameter groups, select an item then press the ✕ button.)
- Once you are finished press **[Select]**.
- Select this new parameter group from the combo box listing the available groups.
- Use the ▶ button to move parameters from the master list into this group. To move several parameters press the <Ctrl> key while you select multiple parameters from the source list, then press ▶ button. To remove parameters from the parameter group, select the target parameter and press the ◀ button.
- Once you are finished in the parameter groups dialogue, press **[Save]** to save the changes and **[Close]** to return to the main menu of AquaChem.



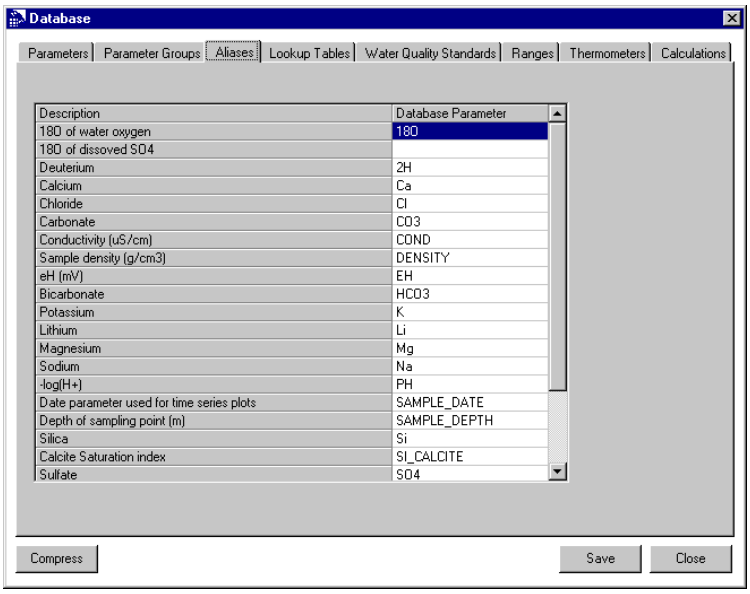
The parameter groups can now be accessed in the **Sample Details** window. To do so, open the details for any sample and you should see the following window:



In the **Measured** parameters tab, beside the **Parameter Group** label, there is a combo box listing the available parameter groups for the database (indicated by the arrow). Simply choose one of the groups from this list, and AquaChem will display only the data for the pre-defined parameters in that group.

3.11.3 Aliases

The third tab in the **Database** dialogue is the **Aliases** tab.

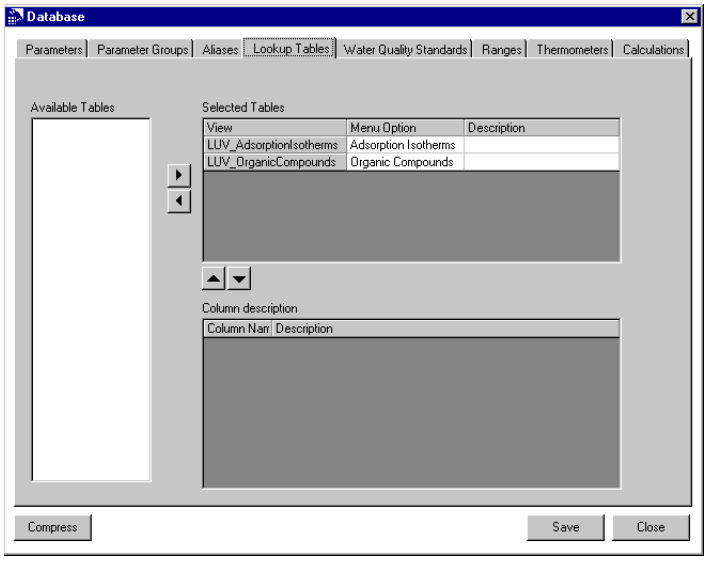


This section allows you to adjust the parameters which are used for some of the internal calculations in AquaChem. Some parameter names have been hardwired to AquaChem for these calculations. For example, in order to calculate the hardness given by the sum of Ca and Mg, AquaChem must know if these parameters are called Ca or CALCIUM in the database. For most purposes, it is highly recommended not to modify the original parameter names. However if you must rename a mandatory parameter, this section gives you the opportunity to map the database field to the parameter name in the database.

Once you are finished in the Aliases dialogue, press **[Save]** to save any changes and **[Close]** to return to the main menu.

3.11.4 Lookup Tables

The next tab in the Database dialogue contains options for **Lookup Tables**, as shown below:



Lookup tables allow you to integrate any type of information in tabular format to the AquaChem Environment which may be helpful for your work. This can be a list of projects, customers, or a table with properties of organic contaminants. These tables are created in the Microsoft Access environment. It is recommended that the table names start with **LUT** (Lookup Table) for the naming convention, (e.g. LUT_organics). Then create a view of this table that orders the data the way you want it to show up in the table in AquaChem. The respective view must start with the letters **LUV** (Lookup Views) in order to be detected by AquaChem.

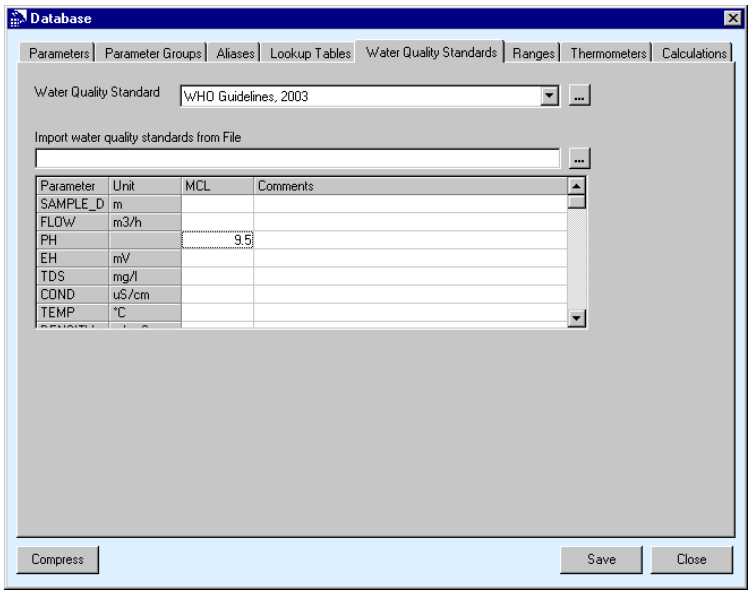
On the left side of this dialogue, you will see **Available Tables** which contains a list of all views starting with **LUV** that are not already integrated into AquaChem. Pressing the ▶ button adds the view to the right-hand grid of **Selected Tables**. The **Menu Option** is the name of the entry as it will appear under the **Tools > Lookup Tables** menu in AquaChem. The **Description** field lets you add a description to the table. The **Column description** allows you to modify the column headings as they will appear in the table.

To access the look up tables, select **Tools > Lookup Tables** from the main menu of AquaChem.

Once you are finished in the **Lookup Tables** dialogue, press **[Save]** to save the changes and **[Close]** to return to the main menu.

3.11.5 Water Quality Standards

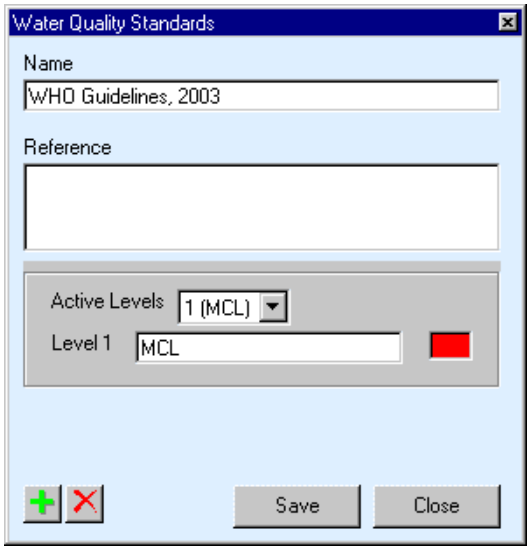
The **Water Quality Standards** options are available under the fifth tab in the **Database** dialogue as shown below:



The options in this dialogue allow you to view and modify water quality standard levels, and create new sets of standards. These standards are used in the data analysis reports, table views, and individual sample details. Measured parameters which exceed these pre-defined levels are flagged as red, orange, or yellow depending upon the specified preferences. This allows you to quickly identify sample exceedances and water samples which may be harmful to humans and the environment.

To view the available standards, simply choose a standard from the combo box beside the **Water Quality Standard** field. Standards can be modified by simply editing the existing values beside each parameter, or importing a complete set of standards from a text file. For each parameter in the database you may define up to three guideline levels.

To view the properties of each Water Quality Standards, press the ... button beside the Standard name, at the top of this dialogue. You should then see the following dialogue:



In this dialogue, you may define the Standard **Name**, **Reference**, **Active Levels**, and names for each **Level**. Or, you can create new standards by pressing the button (this process is explained further below).

Each guideline may have a maximum of three levels; the three levels are colored red, orange, and yellow, and the colors cannot be changed. These colors will correspond to the background of cell values, which are marked for exceeding the respective guideline level:

Values that exceed Level 1 are shaded red;
Values that exceed Level 2 are shaded orange, and
Values that exceed Level 3 are shaded yellow.

These flagged colors will allow you to quickly identify data that exceeds legally enforceable guidelines, and also identify troublesome samples which exceed certain levels, but are classified as tolerable or are aesthetic guidelines only.

The number of levels available is dependent on the guideline used. In most cases, two levels will be adequate (Tolerated level, Guideline level). Simply choose the number of Levels that you want AquaChem to use (choose from 1, 2, or 3 from the combo box beside **Active Levels)**. You may then assign a name to each level (Tolerated level, TCL, cleanup level etc.), Beside the **Level 1** field you may enter your own label for the Level 1 criteria. For example, you can call the first level **MCL** (applicable in U.S.), or you can name this MAC (applicable in Canada). Simply type in the new name in the appropriate field. Similarly, for **Level 2** and **Level 3** you may enter your own labels.

For your convenience, three commonly used Water Quality Standards are included with AquaChem:

- World Health Organization (**WHO**) - Guidelines for Drinking Water Quality - 3rd Edition - 2003
- Canadian Council of Ministers of the Environment (**CCME**)- Canadian Environmental Quality Guidelines - 2002
- U.S. Environmental Protection Agency (**US EPA**) - National Primary Drinking Water Regulations (EPA 816-F-02-013, July 2002).

For your reference, these guidelines are also available in spreadsheet view, and included in your AquaChem installation folder. In addition, the following Water Quality Standard is provided with your installation, and can be imported into AquaChem:

- **US EPA** - National Secondary Drinking Water Regulations (EPA 810/K-92-001, July 1992)

For more details on these standards, please see the website links below:

WHO: http://www.who.int/water_sanitation_health/dwq/guidelines/en/

CCME: http://www.ccme.ca/publications/can_guidelines.html

US EPA http://www.epa.gov/safewater/mcl.html

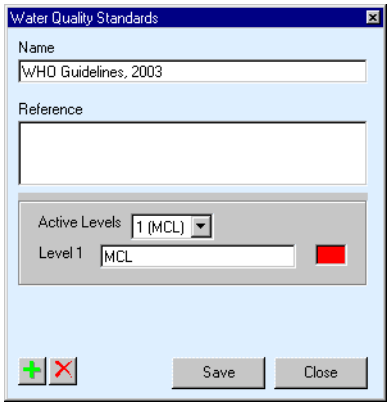
To specify which Water Quality standard should be used for your database, you may do so in the **Preferences** dialogue, available under the **File** menu. Select the **General** tab, and in here you will be presented with a combo box displaying the available Standards.

If the above mentioned standards are not sufficient for your project needs, you may create a new set of standards, as explained in the following section.

Creating New Water Quality Standards

To create a new set of water quality standards, please follow the steps below:

- If you have not already done so, open the **Database** options dialogue (**File > Database**), and select the **Water Quality Standards** tab.
- Press the **...** button (in the upper right corner) to access the Water Quality Standards properties dialogue, as shown below.



- Press the button to create a new standard
- Enter the name for this new set of standards
- Select the appropriate number of Active Levels
- Define a name for each Level
- Press the **[Save]** button, then press **[Close]**

There are two ways to assign the guideline levels to each parameter: the values can be entered manually or the data can be imported from a file. If you elect to enter data manually, proceed to do so for each level for each parameter (or according to the available levels for each parameter).

If you import the data from a file, it is recommended that the parameter names in your text file are identical to the respective parameter names (the Internal Key name) in the database template. If the parameter names are different, AquaChem will not recognize the data for these parameters when you attempt to import them, and you will need to match the fields manually. Please refer to the standards source files (in the WQStandards folder) for an example of the format.

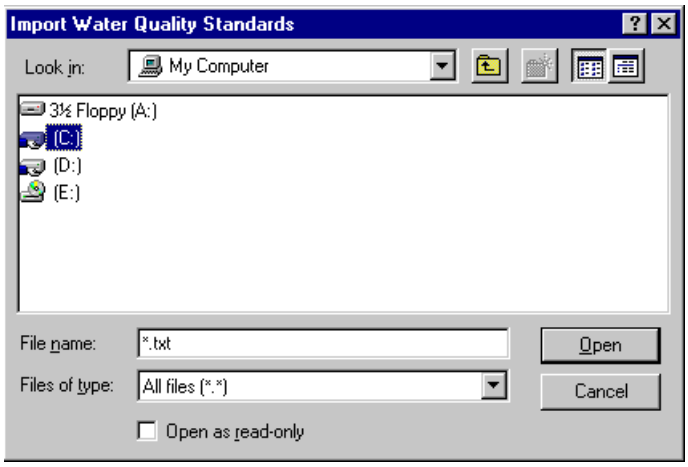
The source file must be a tab-separated .TXT file having the following format:

ParameterName Units Level1 Level2 Level3

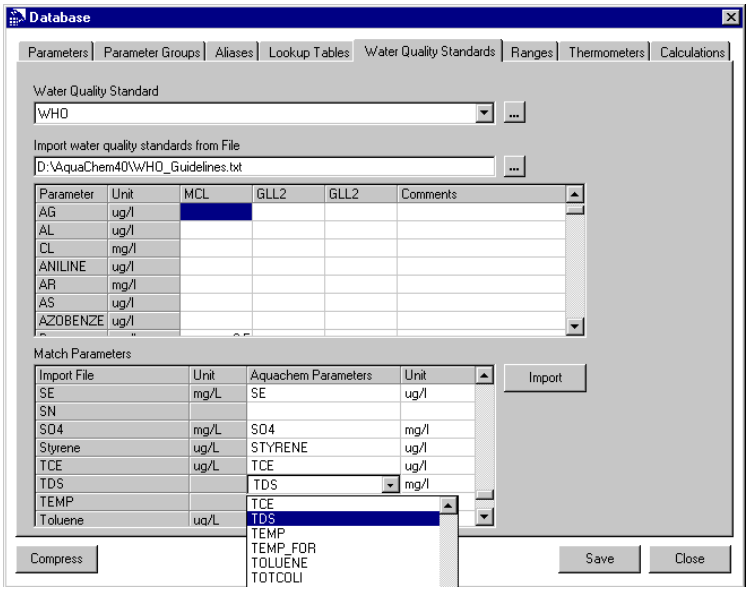
NOTE: Do not include headers in the text file. The first line in your text file should be the first available parameter for which you have a guideline level.

To import the water quality standards using a text data file:

- Press the ... button beside the **Import water quality standards from File** field for the filename. The following dialogue will then appear:



- Locate the source text file on your computer, then press **[Open]**.
- After you load the text file, the dialogue will be refreshed similar to the one shown below:



- At the lower portion of this dialogue, you will see a section labeled **Match Parameters**. AquaChem will attempt to match up the text fields to the

parameters in your AquaChem database. If you see blank fields, then this indicates that the fields were not recognized by AquaChem and you will need to match up the fields manually. To do so double-click in the parameter field, and choose the matching parameter from the combo box (as seen above for TDS). Do this for each 'missing' parameter field.

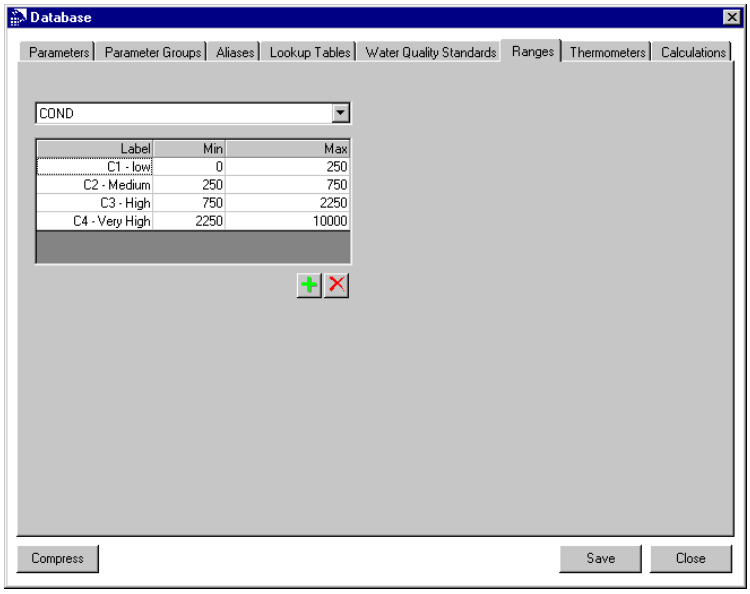
- You must also specify the units for the guideline level. The units that may be used are: mg/L, ug/L, ppm, ppb. The unit to be imported depends on the unit of the respective parameter in the database. For example, if Fe is saved in ppm then the imported units can only be ppm or ppb, same for mg/L and ug/L.
- Once you are finished, click the **[Import]** button.

The new data will now be added to upper portion of this dialogue for the selected Water Quality Standard. To use this new standard, you must select this in the **File > Preferences** dialogue, under the **General** tab.

Once you are finished in this dialogue, press **[Save]** to save the changes and **[Close]** to return to the main menu.

3.11.6 Ranges

The next tab in the Database options is the **Ranges** tab, as shown below:



Ranges are similar to the drinking water standards; they allow you to define named intervals for any parameter. An example for Conductivity (COND) is shown in the dialogue above, and detailed below:

Conductivity (uS/cm)	
<250	low salinity (C1)
250-750	medium salinity (C2)
750-2250	high salinity (C3)
>2250	very high salinity (C4)

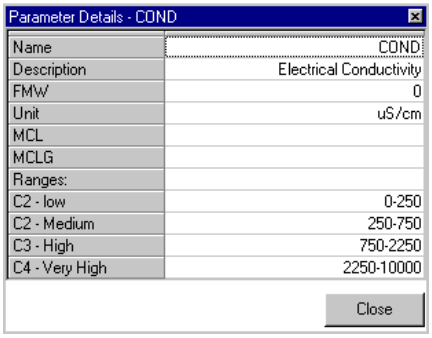
Ranges can be useful for interpreting stable isotope data: S, N, C, Sr, He. Isotopes reflect the signature of their source. If the ranges of every potential source is given, an analyzed value can easily be attributed to one of the sources. The range definition can be used with the range_name function in the Report Designer. For example, the range name (pH) will return the name of the respective interval name in which the current pH value is included.

Creating a New Range

To add a new Range item:

- Choose the desired parameter from the combo box at the top of this dialogue.
- Press the  button to add a new item.
- Enter the desired **Label** (descriptive name or text).
- Enter the corresponding **Minimum** and **Maximum** values.
- Press **[Save]** to save the changes and **[Close]** to return to the main menu.

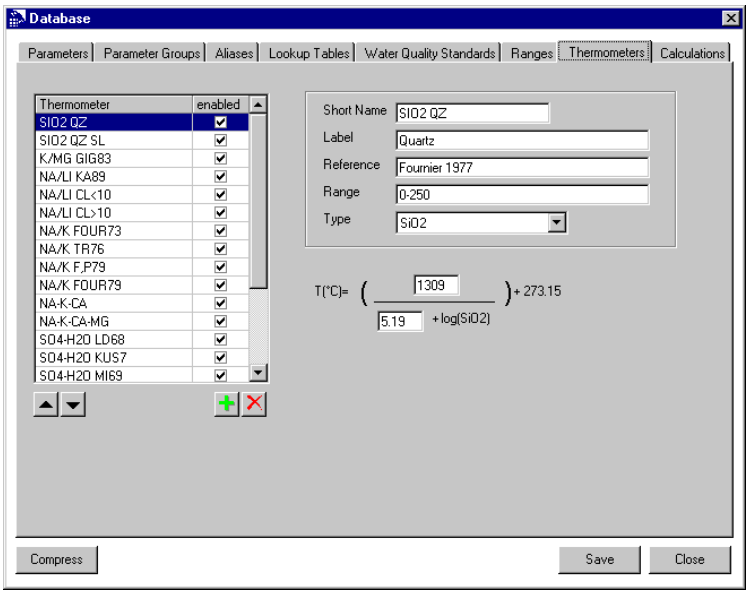
To view the range options for a sample, load a **Sample Details Window** and then ***right-mouse click*** on the parameter name. A dialogue titled **Parameter Details** appears, showing all the information about this parameter including the ranges.



The Range information should appear in the lower section of this dialogue.
Once you are finished in this dialogue, press **[Save]** to save the changes and **[Close]** to return to the main menu.

3.11.7 Thermometers

The next tab in the **Database** options dialogue is the **Thermometers** tab, as shown below:



The Thermometers options allow you to modify existing Geothermometers or to create new ones. Geothermometers are used to estimate the original subsurface reservoir temperature of ascending groundwater which underwent conductive cooling during its ascent. They reflect the temperature dependence of most rock-water reactions. The reactants, which remain dissolved during the journey to the surface, are ideally proportional to their original aquifer temperatures. For example SO_2 (Quartz or Chalcedony dissolution or Na/K for albitisation). The original reference and the temperature range for which the thermometer is valid (most thermometers only work above 100 °C) and can be viewed and edited in this dialogue.

Geothermometers are generally derived from the Van't Hoff equation and have the form:

$$T(^{\circ}C) = \left(\frac{a}{b + \log(K)}\right) + 273$$

where

a and *b* are constants describing a straight line in the 1000/T-log(*K*) plot, and

K depends on the reaction used for the geothermometer (SiO_2 for all SiO_2 thermometers, Na/K for the Na/K thermometer, etc.)

Since thermometers are usually developed from empirical data, different coefficient values are found in the literature. AquaChem includes a compilation of most currently used geothermometers as shown in the figure above. The equations for each of the thermometers are stored in the project database file and can be customized and modified. Each thermometer record includes the formula's coefficients, the reference (author and year), and the range within which the formula was calibrated.

The **Thermometers** tab contains a list of available geothermometers that can be plotted on a geothermometers plot. If a thermometer is enabled (checked) it will be available for the geothermometers plot. If it is disabled (not checked) it will not be available for the geothermometers plot.

There are several fields for each thermometer:

- The **Short Name** refers to the list name of the selected geothermometer.
- The **Label** refers to the reference name of the geothermometer.
- The **Reference** refers to the author and year of the original publication.
- The **Range** refers to the temperature range within which the thermometer is supposed to provide reliable data. This normally corresponds to the range of the calibration data.
- The **Type** refers to the thermometer class.

Creating a New Geothermometer

You may add published thermometers from literature or create your own thermometer if the formula structure corresponds to one of the pre-defined thermometers provided by AquaChem.

For example, to create a new Na/K thermometer:

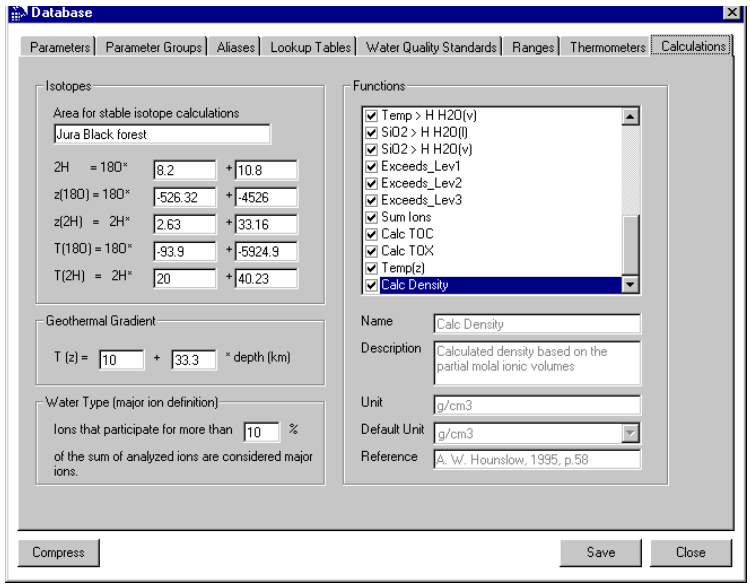
- Select an existing Na/K geothermometer,
- Click the  button to create a new Na/K geothermometer.
- Select the new geothermometer **Type**.
- Enter a new **Short Name**, **Label**, **Reference**, and **Range**.
- Replace the formula parameters from the original geothermometer with the parameters from the new geothermometer.
- Press the **[Save]** button to save the changes to the database.

This new thermometer is automatically included in thermometer calculations and can be visualized as a **Geothermometer Plot**.

Once you are finished in the Thermometers section press **[Close]** to return to the main menu.

3.11.8 Calculations

The last tab in the Database options dialogue is the **Calculations** tab, as shown below:



The **Calculations** tab allows you to set the equation coefficients and parameters that are used in the isotope and geothermometer calculations. It also provides information on the various calculations that are performed by AquaChem.

Isotopes

In the **Isotopes** frame, you may define coefficients for several functions for the isotopic calculations. With the exception of the meteoric water line, all equations have a highly regional character. If you want to make temperature or precipitation estimations, please find the respective coefficients for your study area. There are also parameters for ^{18}O (Oxygen 18) and ^{2}H (deuterium) equations: meteoric waterline, altitude-isotope and altitude-mean annual temperature relations. All of these functions are derived empirically. The coefficients for the isotope-altitude and the isotope-temperature functions are regional and should be used only in the area of calibration. Indicate the area of application of these functions in the field provided.

Geothermal Gradient

The **Geothermal Gradient** is used for a simple subsurface temperature estimation. These options allow you to specify which values are used to calculate the temperature at a given depth. The geothermal gradient is used in the geothermometer plot. It allows

the user to estimate the subsurface temperature of waters produced by a borehole if the depth of the inflow zone is known. This temperature is then compared to geothermometer temperatures for the respective sample.

The formula for the Geothermal Gradient calculation is as follows:

The subsurface temperature [T (z)] = Average surface temperature + geothermal gradient * depth (km).

The geothermal gradient may vary regionally; it is approximately 33 °C/km in most environments. Any changes made to the Geothermal gradient equation should be registered with AquaChem by pressing the **[Save]** button prior to closing the **Database** options dialogue.

Water Type (major ion definition)

The criterion for determining if an ion is major is normally 10%; however in some places 12.5% is more common. This option allows you to enter a new value for the major ions calculations definition. This will influence the water type calculation which is based on the major ions.

Water type is calculated as follows:

- All concentrations are converted to meq/L.
- Values are then transformed from meq/L to meq%.
- All parameters which are below a certain limit (10% by default) are removed.
- The remaining ions are considered **Major ions**. These ions are ordered according to their percentage. Cations are ordered first, followed by the anions.
- The result is the **WaterType** string (e.g. Ca-Mg-HCO_3).

The Water Type is displayed in the **Sample Details** window as a distinct parameter.

NOTE: The Water Type parameter cannot be edited; it is read-only.

Functions

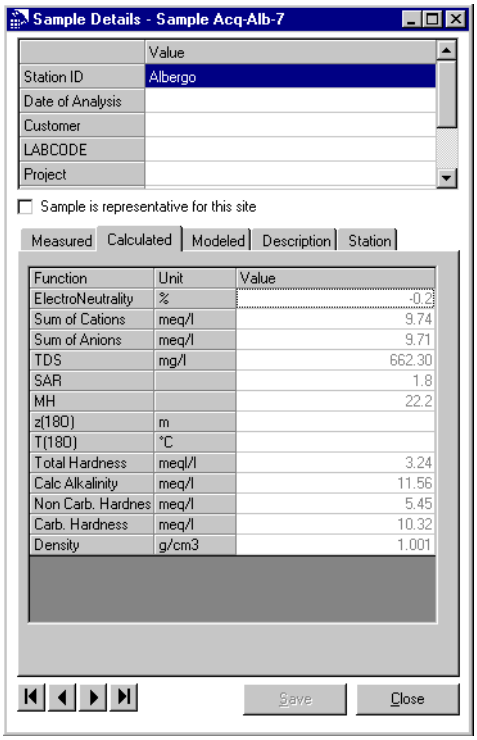
The **Functions** frame lists all of the internal calculations performed by AquaChem, with reference information for each calculation provided in the fields below. All of the active functions (as indicated by a checkmark) will be available as database parameters which can be included in statistical comparisons and for plotting data. In this dialogue, you may select which calculations should appear in the function lists. For example, if you never use the enthalpy calculation, you may deactivate it here. In addition, you may define the default units for some of the functions.

The calculated values are displayed in the **Sample Details** window, under the **Calculated** tab:

The functions such as hardness, ion balance, etc. are hardwired to AquaChem; as such, it is not possible to change the parameters involved in these calculations. You may however, edit the name of the function or activate or deactivate a function. Deactivated functions will not appear in the list of functions within AquaChem. For functions that can be expressed in different units (e.g. hardness, °F, g, mg/L $CaCO_3$) you may specify the default unit.

To edit the name of the function, press **View > Options** when the Sample Details window is active, and edit the options under the **Functions** tab.

AquaChem includes a number of common calculations for determining common geochemical parameters. Each of the available calculations (functions) is explained below.



Calculated Alkalinity

Acid neutralizing capacity. Generally equal to the concentration of CO_3 + HCO_3 + H_2CO_3.

Calculated Density

Calculated density based on the partial molal ionic volumes. This value is calculated as follows:

$$D = \frac{\left[1000 - v + \frac{TDS}{1000}\right]}{1000}$$

where

v is the molar volume: $v = \Sigma(n_i \cdot v_i)$,

n_i is the concentration in mmol/l of ion i and,

v_i is the partial molar volume at $25°C$

Partial molal ionic volume coefficients are from Owen and Brinkley, 1941 and for more details, see Hounslow, 1995, p. 58

Calculated TDS (Total Dissolved Solids)

TDS is a measure of the evaporation residue at a given temperature. It can also be thought of as the mass of all ions. It is important to note that the calculated TDS is only an approximation and it is always better to have a measured value.

TDS is calculated as follows:

First the sum in mg/L of Na+K+Mg+Ca+Cl+SO_4 is calculated. Then AquaChem checks if (Ca+Mg-SO_4) > (HCO_3+CO_3). This is done because TDS is not simply the sum of ions but the weight of residue you would expect if you evaporate the entire sample. In waters that contain an excess carbon (Ca+Mg-SO_4) < (HCO_3+CO_3) you may not add all carbon since bicarbonate will partly outgas as CO_2 during evaporation. Only the quantity of HCO_3 which can be precipitated as calcite and dolomite is added to the estimate of the TDS. SO_4 is deduced from Ca+Mg because gypsum is built first and the Ca that is used up by this process cannot be used any more to build calcite. If (Ca+Mg-SO_4) > (HCO_3+CO_3) then all HCO_3 and CO_3 can be added to the TDS because there is enough Ca+Mg to build calcite and dolomite.

Total Hardness

The sum of ions that can precipitate from water as hard particles. Generally, the sum of Ca and Mg, expressed in meq/L or mg $CaCO_3$/L, or in degrees.

100 mg $CaCO_3$/L = 1 mmol Ca^{2+}/L = 2 meq Ca^{2+}/L

The Degrees equivalents are as follows*:*

1 German Degree = 17.8 mg $CaCO_3$/l

1 French Degree = 10 mg $CaCO_3$/l

Non Carbonate (Permanent) Hardness:

Parts of Ca and Mg in excess of HCO_3.

Carbonate (Temporary) Hardness:

Parts of Ca and Mg which are balanced by HCO_3 and thus can precipitate as $CaCO_3$.

ElectroNeutrality

(Cations - Anions)/(Cations + Anions), expressed as a percent.

Sum of Anions:

Sum of all measured anions for the sample, in meq/l.

Sum of Cations:

Sum of all measured cations for the sample, in meq/l.

Sum Ions:

Sum of all ions in your sample. This can be expressed in mmol/l, meq/l, mg/L.

Exceeds_Lev1, Exceeds_Lev2, Exceeds_Lev3

The functions “Exceeds_Lev1, Lev2, Lev3” may be used in the Find utility. If you have multiple samples it is very convenient to search for all samples that exceed one of the levels of the currently defined water quality standards, and mark them in the open plots. This is especially effective if you are dealing with many different parameters that might exceed the guidelines. The function Exceeds_Lev1 returns true if one of the concentrations of the current sample exceeds the level 1 of the active water quality standard, Exceeds_Lev2 returns true if the sample contains values that exceed level 2, etc.

SAR (Sodium Adsorption Ratio)

$$SAR = \frac{Na}{\left(\frac{Ca + Mg}{2}\right)^{0.5}}$$

NOTE: The Concentrations used in the formula are in meq/L.

MH (Magnesium Hazard)

Magnesium is considered to be harmful for plants, but the effect is reduced by the presence of calcium. Magnesium Hazard was proposed by Szabolcs and Darab (1964).

$$MH = \frac{Mg}{(Ca + Mg)} \times 100$$

Units are in meq/l. MH > 50 is considered to be harmful for irrigation water.

NOTE: The Concentrations used in the formula are in meq/L.

Calculated TOC

Calculated Total organic carbon. Sum of carbon present in ug/L, mg/L or g/L in all organic parameters. Therefore, carbon from HCO_3, CO_3, CO_2 is not included.

Calculated TOX

Calculated total organic halogens. Sum of all halogens (e.g. Cl^-, Br^-, I^-, etc.) present in ug/L, mg/L or g/L in all organic parameters (thus, Cl from Cl^- or CL2 is excluded).

z(18O)

Average infiltration height as a function of oxygen 18 isotopic composition. Coefficients are valid only for a very limited zone, and must be established using empirical data. This also requires the coefficients of the equations which describe the altitude and temperature isotope relation.

T(18O)

Average temperature of infiltration zone as a function of oxygen 18, isotopic composition. Coefficients are valid only for a very limited zone, and must be established using empirical data. This also requires the coefficients of the equations which describe the altitude and temperature isotope relation.

T(2H)

Average temperature of infiltration zone as a function of deuterium. Coefficients are valid only for a very limited zone. This also requires the coefficients of the equations which describe the altitude and temperature isotope relation.

z(2H)

Average infiltration height as a function of deuterium. Coefficients are valid only for a very limited zone. This also requires the coefficients of the equations which describe the altitude and temperature isotope relation.

Temperature (Z)

Estimated Temperature for a given depth and geothermal gradient.

Temp > H H2O (l)

Enthalpy of liquid water as a function of temperature (*t*). This is a polynomial function:

Temp = *enth(water)*

value! = *a(1) + a(2) * t + a(3) * t ^ 2 + a(4) * t ^ 3 + a(5) * t ^ 4 + a(6) * t ^ 5 + a(7) * t ^ -1 + a(8) * t ^ -2 + a(9) * log10(t)*

where

a(1) = 418.84

a(2) = 10.286

a(3) = -0.05092

a(4) = 0.00026309

a(5) = -0.00000069303

a(6) = 0.00000000074566

a(7) = -1209.8

a(8) = 11.99

a(9) = -353.76

For more details please refer: Fournier & Potter, 1972.

Temp > H H2O (v)

Enthalpy of water vapor as a function of temperature. This is a polynomial function:

Temp = *enth(water vapor)*

enthalpy = *a(1) + a(2) * t + a(3) * t ^ 2 + a(4) * t ^ 3 + a(5) * t ^ 4 + a(6) * t ^ 5 + a(7) * t ^ -1 + a(8) * t ^ -2 + a(9) * log10(t)*

where

a(1) = 2035

a(2) = -5.0499

a(3) = 0.057399

a(4) = -0.00030426

a(5) = 0.00000079095

a(6) = -0.00000000086968

a(7) = 1342.4

a(8) = -13.298

a(9) = 396.29

For more details please refer: Fournier & Potter, 1972:

SiO2 > H H2O (l)

Enthalpy of liquid water as a function of dissolved silica. This is a polynomial function:

enth = *a(1) + a(2) * SiO2 + a(3) * SiO2 ^ 2 + a(4) * SiO2^ 3 + a(5) * log10(SiO2)*

where

a(1) = -42.198

a(2) = 0.28831

a(3) = -0.00036686

a(4) = 0.00000031665

a(5) = 77.034

For more details please refer: Fournier & Potter, 1972:

SiO2 > H H2O (v)

Enthalpy of water vapor as a function of dissolved silica. This is a polynomial function:

enth = *a(1) + a(2) * SiO2 + a(3) * SiO2 ^ 2 + a(4) * SiO2^ 3 + a(5) * log10(SiO2)*

where

a(1) = -3.5532

a(2) = 0.146

a(3) = -0.0004927

a(4) = 0.0000012305

a(5) = -0.00000000049421

For more details please refer: Fournier & Potter, 1972:

The calculated parameters are treated by AquaChem as regular database parameters with respect to plotting, searches, or statistical calculations. However, in order for the built-in calculations to work, their corresponding database parameters must be included in the database. For example, the database must include Ca and Mg in order to calculate

hardness, and both of these parameters must be identified with an Internal Name of ‘Ca’ and ‘Mg’ respectively.

> **NOTE**: If your database does not include some of the required parameters or if some of the required parameters are not properly named, then the applicable function(s) requiring these parameters will contain null values or erroneous information.

Once you are finished in the Calculations section, press **[Save]** to save the changes and **[Close]** to return to the main menu.

4

Plots

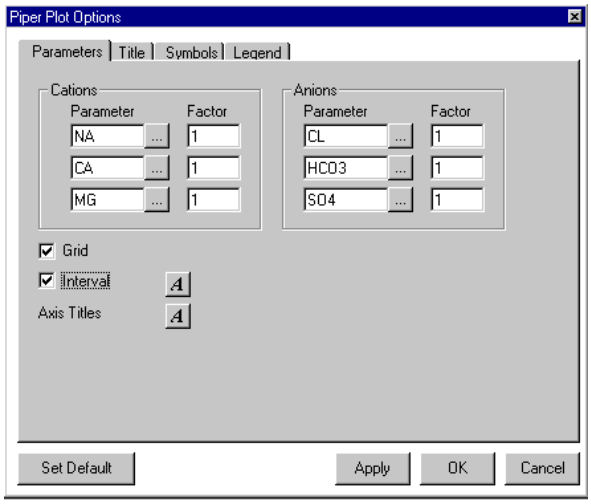
When you select **Plots** from the main menu and then **New**, a drop-down menu will appear with a list of the seventeen (19) available plot types:

- Box and Whisker (Multiple Parameters)
- Box and Whisker (Multiple Stations)
- Depth Profile
- Durov Plot
- Geothermometer Plot
- Giggenbach Triangle
- Histogram
- Ludwig-Langelier Plot
- Map Plot
- Pie Plot
- Piper Plot
- Radial Plot
- Scatter Plot
- Schoeller Plot
- Stiff Plot
- Ternary Plot
- Time Series Plot (Multiple Parameters)
- Time Series Plot (Multiple Stations)
- Wilcox Plot

AquaChem allows you to create multiple plots for the same data set and view these plots simultaneously within the Windows environment. Each of these plots is explained in greater detail later in this chapter. The following section describes some of the features that are common to all plots.

4.1 Common Plot Features

Although each graph type has unique characteristics, there are also many graphical features and options that are common for each one. When you select any of the graph types to plot, a **Plot Options** dialogue similar to the one below, will appear with default settings for the necessary parameters and plot settings.



After the plot has been created, there are two ways to access the **Plot Options** dialogue:

- Click **View** from the main menu and then **Options** when a plot window is the active window; or
- ***Right-mouse*** click on the **centre** of the plot window.

The **Plot Options** dialogue is typically divided into four tabs: **Parameters**, **Title**, **Symbols**, and **Legend**.

Parameters Tab

Contains information on the parameters/series used in the plot, axis labels and font options, axis titles and ranges, and toggles to turn the plot gridlines or axis ticks on/off.

Title Tab

Contains options for plot title, position, and font size.

Symbols Tab

Contains options for symbols used in the plot, symbol labels, proportional symbol options, etc.

Legend Tab

Contains options for displaying a plot legend, legend title, and display features.

Each **Plot Options** dialogue has the following buttons located at the bottom of the dialogue:

The **[Apply]** button will apply the current plot settings to the selected plot type.

The **[OK]** button will apply the current plot settings to the selected plot type and will close the plot options dialogue.

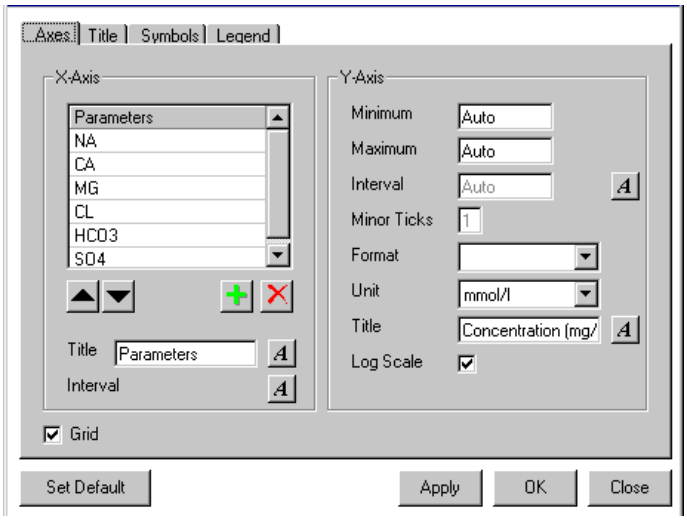
The **[Cancel]** button closes the plot options dialogue.

The **[Set Default]** button will save the current plot settings as defaults for that plot type. This includes plot parameters, grid lines, interval, axes titles, legend appearance and symbol settings, but does not include plot titles. The default settings will be applied every time you create a **NEW** plot of that type, with the current database.

Each tab in the plot options dialogue is explained in greater detail in the following section.

4.1.1 Parameters/Axes Tab

Depending on the plot you select, the first tab in the plot options dialogue will be called **Axes** or **Parameters**.



Since the triangular plots (Piper, Durov and Ternary) do not have typical axes, the corresponding tab is labelled as Parameters instead of Axes.

In this tab, you can select the parameters which are used for the plot, the plot axes, maximum and minimum values, axis titles, fonts, and display formats.

The **Axes/Parameters** tab has several buttons and functions which are common for most (but not all) plot types:

The add button allows you to add new parameters to the plot. The add button will load the parameter list dialogue, and allow you to select a new parameter from the list of available parameters in your database. Simply choose the desired parameter, press the **[Select]** button and this parameter will be included in the plot.

The delete button will remove the selected parameter from the plot parameters list.

The up-arrow button allows you to shift the selected parameter upwards in the list of parameters.

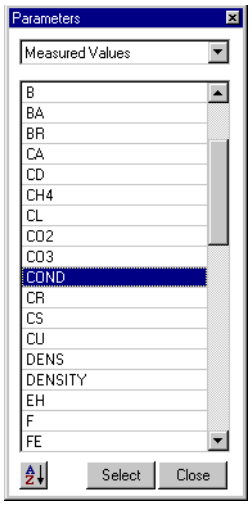
The down-arrow button allows you to shift the selected parameter downwards in the list of parameters.

The font button allows you to edit the font for the current text item (i.e. plot title, axis title, labels, and intervals).

This button will load **Parameters** dialogue with the parameters list (read from your database template) as shown and described below.

Parameters

Most **Plot Options** dialogues have several fields for assigning chemical or physical parameters. These parameters can be typed directly into the text fields or selected from the **Parameters** dialogue (right).



From the top of the **Parameters** dialogue, you can choose the parameters category (Measured, Calculated, Modeled, and Thermometers). Then highlight the new parameter from the list, and press the **[Select]** button. This parameter will replace the existing plot parameter. Most of the parameter fields can also accommodate operators and functions (e.g. Na+K or Na/Cl). Simply enter these functions manually into the parameter field. However multiple parameters (e.g. Na,Cl) are not accepted.

NOTE: The parameters category may be pre-defined for some plots. Also, some plots have pre-defined parameters which cannot be modified. As such, the parameter field for these plots will be greyed out and will be read-only.

Once you are finished, press the **[Close]** button to return to the plot options dialogue.

Minimum/Maximum

Allows you to customize the minimum and maximum axes values. AquaChem will determine a default minimum/maximum value based on all of the data plotted on the graph. If you enter a new value and you wish to return to automatic calculation, enter "A" in this field.

Labelled Ticks / Interval

Defines the interval value of the labelled ticks for the corresponding axis. AquaChem will determine a default value for the labelled ticks such that the plot will have 5 labelled ticks on the corresponding axis. If you enter a new value and you wish to return to automatic calculation, enter a value of "A" in this field.

Minor Ticks

Defines the number of minor ticks between each of the labelled ticks. The default value is 1. Only integer values are accepted.

Format

Sets the numeric format for the labels on the axes (e.g. Auto, 0, 0.0, 0.00, 0.0E+00, etc.). Beside **Format**, click  button in the combo box to select from the list of available numeric formats.

Title

Defines the title of the corresponding axis. If a title field is left empty, a default title equal to the internal name of the parameter will be selected by AquaChem. If you want to omit one or both axes titles, type a space in the text field(s).

Units

Defines the units for the parameters that will be plotted on the selected graph (mg/L, mmol/L, mol/L, meq/L, ppm). AquaChem will perform an automatic unit conversion on each data point before it is plotted on the graph.

Fonts

The default fonts for axes title and labels can be modified by selecting the  button. The Font dialogue provides a selection of all available Windows true type fonts, font sizes and font styles.

Log Scale

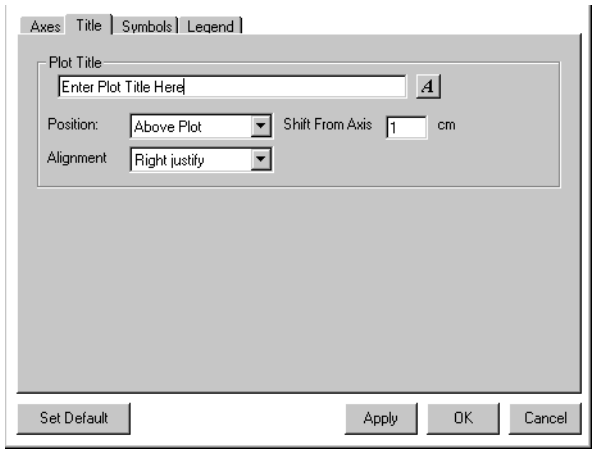
Some plots allow you to show the plot data using a log scale for either the X or Y axis, or both. This allows you to normalize the data set, if there is a significant range in the data.

Grid

Displays gridlines on the plot with the same interval as the labelled ticks.

4.1.2 Title Tab

For most plot types, the second tab in the plot options dialogue is **Title**.



In this tab, you can enter a **Plot Title** and edit the title font by pressing the A button. In addition, you can change the **Position**, and **Alignment** of the plot title.

Plot Title

Defines the title of the selected graph type. Enter the plot title in the text field provided. If no text is entered, then no title will be plotted.

Position

Defines the position of the Plot Title as either **Above Plot** or **Below Plot**.

Alignment

Defines the alignment of the Plot Title as either **Left justify**, **Centre justify**, or **Right justify** in the plot window.

Shift From Axis

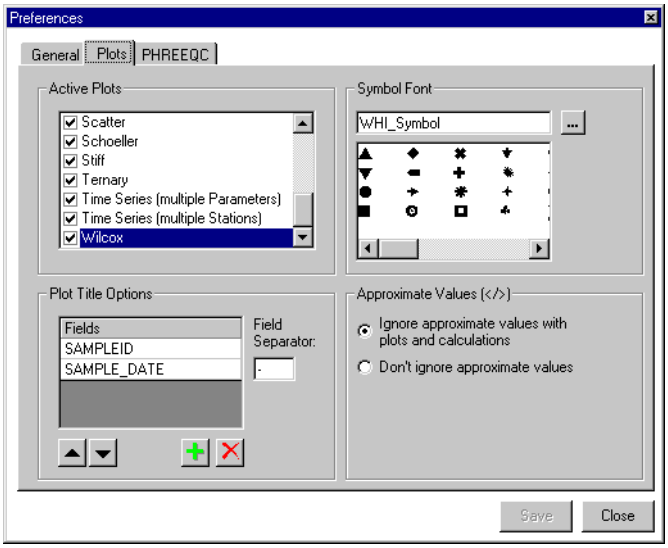
Defines the vertical distance of the Plot Title above or below the plot.

Automatic Plot Title Option

AquaChem v.4.0 includes a useful utility which will allow you to automatically assign plot titles based on any station or sample description parameter, or a combination of these parameters. This is very practical especially when you are creating a large number of plots.

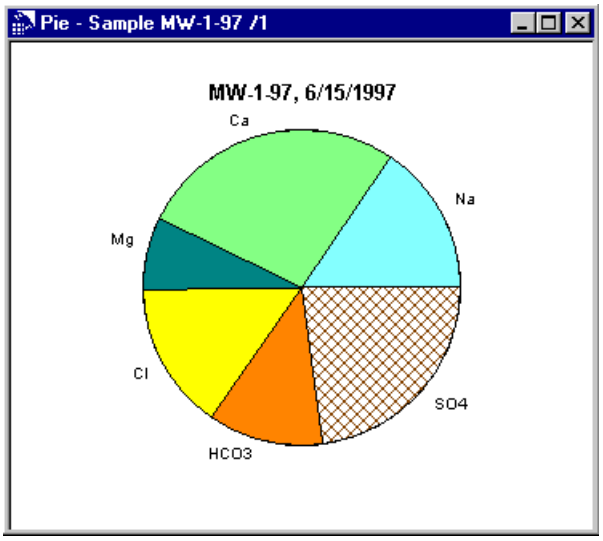
NOTE: This feature is applicable only to plot types that represent one distinct sample per plot (**Pie, Radial** and **Stiff** plots only).

To setup the Automatic Plot Title features, close all plot windows and ensure the sample list is the active window. Select **File** from the main menu, then **Preferences**. From this dialogue, choose the **Plots** tab and a window similar to the one shown below will appear.



Under the **Plot Title Options** section (in the lower-left corner), you can specify which parameters you would like to appear when using the automatic title option. Parameters can be arranged, and added/removed using the up, down, add, or remove buttons. Once you are satisfied with the parameters, you must specify a **Field Separator**. This will be the character that separates the parameters in the title of the plot. You can use any character as the field separator, however the most common are a hyphen, comma, or semi-colon.

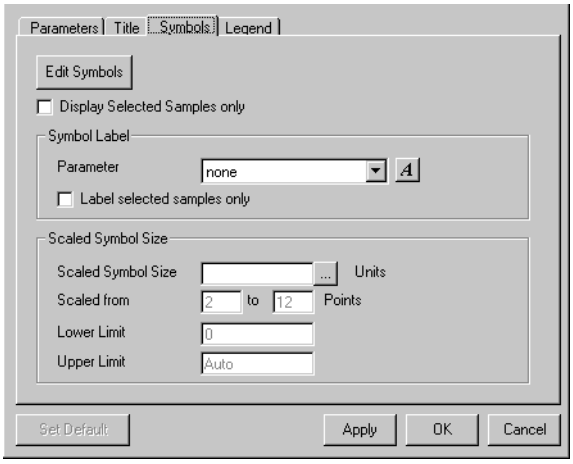
Using these parameters above, you can see an example below of a Pie Plot which is created with the automatic title option:



NOTE: By default, all **Pie**, **Radial**, and **Stiff** plots will be titled automatically with the fields specified in the **Preferences** dialogue. To change the plot title after the plot has been created, simply type in a new plot title in the **Plot Title** field, and press **[OK]**.

4.1.3 Symbols Tab

For most plots, the third tab in the Plot options dialogue will be **Symbols** as shown below. These options allow you to edit the symbol options as they appear on the plot.



Edit Symbols

The **[Edit Symbols]** button opens the **Define Symbol or Line** dialogue. In this dialogue, you can define the names and status of the symbol groups, the shape and color of the symbols, and the line-type and color of lines that appear in the plots (refer to the **Define Symbol or Line** section in Chapter 3 for a description of the symbol groups settings).

Display Selected Samples only

When this option is selected, the plot will display only those samples which are highlighted in the active sample list. If this option is not selected, then the plot will display all samples which are in the active sample list.

Symbol Label

This option allows you to specify a parameter to be used as a symbol label on the plot. You may choose from Station Description or Sample Description parameters. This option allows you to quickly identify samples in the plot.

Label Selected Samples only

If a parameter has been defined for a symbol label, this option can be used to label just those samples which are selected (i.e. highlighted) in the active sample list. If this option is not selected, then all samples will be labeled in the plot.

Scaled Symbol Size

This option allows you to scale the size of plot symbols based on a user-defined parameter (TDS, pH, COND, for example). This allows you to add an additional parameter to your plot. For example, in a Scatter plot, you can display information on three parameters, instead of only two (X-Y) parameters. Once the parameter is selected, you can choose different units for this parameter.

Symbol Size (points)

Defines the minimum and maximum radius of the scaled symbol size. The minimum symbol size will be plotted for the lower limit of the proportional parameter value, while the maximum symbol size will be plotted for the upper limit of the proportional parameter value. The minimum radius ensures that all symbols will be visible even if the proportional parameter value is zero.

Lower and Upper Limit

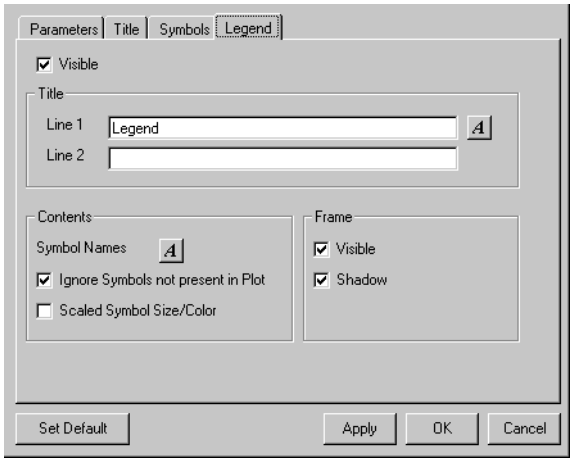
Defines the minimum/maximum value of the proportional parameter to use for plotting a proportional symbol size. The lower limit is the value below which the symbol size

does not get any smaller; i.e. all samples with a proportional parameter value less than the lower limit, will use the smallest symbol point size; likewise for the upper limit. The purpose of the lower limit is simply to set a value below which the symbol sizes do not change.

If you want to exclude symbols from the plot based on a specified criteria, then you should create a query to filter out the undesirable samples.

4.1.4 Legend Tab

For most plots the last tab will be **Legend**.



Visible

To turn the Legend on, place a check mark in the box beside **Visible**. This will display a legend on the right-hand side of the plot listing all of the active symbol groups and the associated symbol shape for each.

Title

The legend title can be entered in Line 1 and Line 2 (optional) and the font for the title can be edited by pressing the A button.

Contents

When the legend is visible, the **Symbol Names** from the currently selected symbol group will be displayed on the plot. The font button beside the Symbol Names allows you to edit the font of the symbol names as they appear in the legend.

Ignore symbols not present in plot

When this option is active, the plot will show only those symbols which are used in the current plot. For example if 10 symbols are active, but the current selection of samples only uses 2 of them, AquaChem will ignore those symbols that are not present in the plot and display just the 2 symbols in the legend.

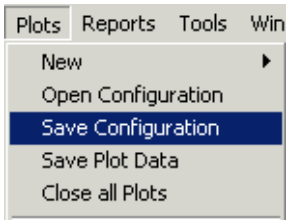
Scaled Symbol Size/Color

This option is only active if you have symbol sizes plotted proportional to a parameter value, under the **Symbols** tab. When this is activated, the legend will show a scale for the proportional symbol sizes.

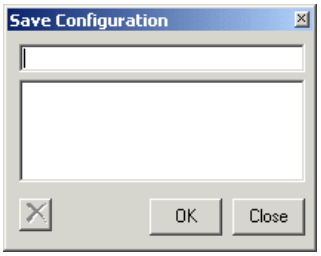
Frame

Activating **Visible** and **Shadow** options will place a rectangular frame around the legend contents, and a shadow effect around the frame.

4.2 Plot Configurations



Once you have created the desired plot, or combination of several plots, the **Save Configuration** option under the **Plots** menu is enabled. This allows you to save the current configuration of open plots and their settings, to your database.
The configuration includes axis settings, selected samples, symbol settings, etc.



When you select **Save configuration**, the dialogue shown on the right side will appear prompting you for a name for the Plot Configuration. Simply type in a name for the plot configuration.
Once you are finished, click **[OK]**.

To recall a saved plot configuration in the future, use the **Plots > Open Configuration** option. Simply select the plot configuration you desire, then click **[OK]**. This will load the plot(s) and their settings. When a plot configuration is loaded, the sample selection used for this plot will also be reset in the Active List window. To remove any unwanted or outdated plot configurations, simply select the respective item from the list, and press the button. Once you are finished, click **[Close]**.

NOTE: The plot configuration files can only be loaded in the AquaChem database in which they were created.

4.3 Save, Show, and Identify Plot Data

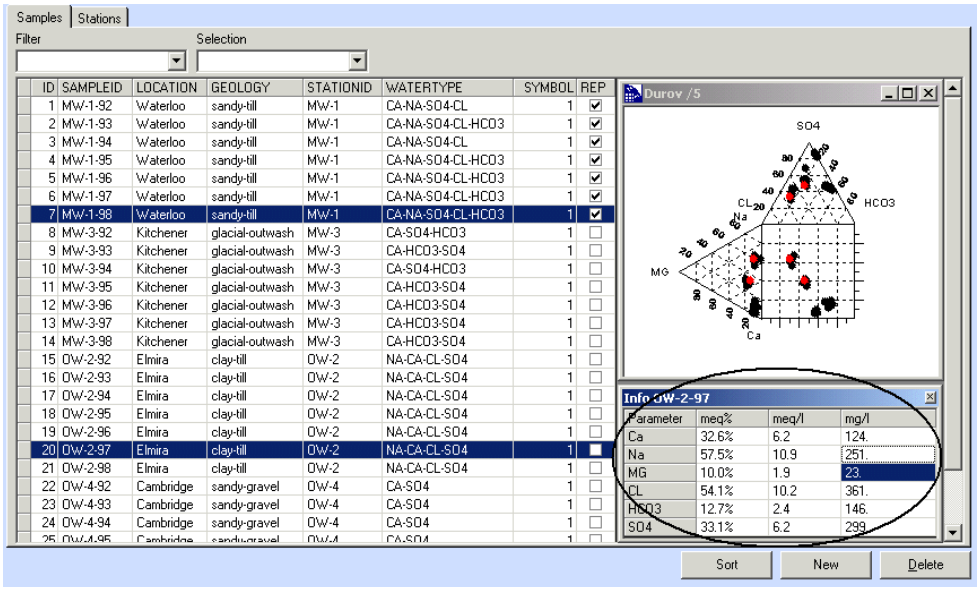
Save Plot Data

When you select this option from the **Plots** menu, a new dialog will open containing a worksheet displaying the plot data of the current plot. This feature is useful if you want to use another plotting program. This menu item is only active when a plot window is loaded.

To save the data choose **Save** from the **File** menu; the data can be saved as .TXT or .CSV format.

Show Sample Data

If this option is selected from the **Plots** menu, AquaChem will display a small dialogue with the data for the selected sample. Simply click on a sample point from the plot and the **Info** data dialogue will appear. Each time you click on a new sample point, the new data is loaded into dialogue. An example is shown below:



NOTE: You may need to re-arrange the positions of your windows in order to see the Sample Data dialogue.

Identify Plot Data

The Identify option allows you to link the plotted data to the samples in the active list. This allows you to click on a point in the graph and view the corresponding sample in the active list. This is useful when you have a large number of samples plotted on one plot, and you want to identify outliers.

There are three options available for selecting and identifying points on a plot: **None**, **Selected Plot**, and **All Plots**. The default mode to identify points is on All Plots; this means that all data points on all plots are linked to the database. These three options are described below:

None

If this option is selected, then no symbols will be highlighted on the plot when the samples are selected. The data points on the graphs are not linked to the database which means that samples are not identified. When you have several open graphs and a large database with many samples, it may be convenient to have no link between the graphs and the database in order to increase the speed of the various AquaChem operations.

Selected Plot

Only the data points in the active graph are linked to the database. The plotted point is activated (turns red) and is selected in the sample list. This mode is useful if you are working with a large data set and want to focus on just one graph.

All plots

The sampling point of the corresponding sample is activated on all plot windows and on the sample list. If you are working with several graphs, you can identify a sample in all plots as well as in the sample list by clicking near a point in any of the plots, or by clicking on a sample in the active list. The sample will become selected in the active list, and the corresponding data points will be highlighted in red in all the open plot windows.

4.4 Printing and Exporting Plots

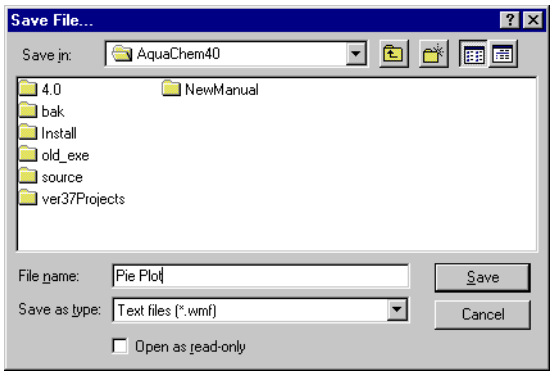
Once you are satisfied with your plot(s) and their design, you have three options for producing output:

- The plot can be saved as a Windows Metafile (.WMF) and printed from an external application, or inserted into a report;

- The plot can be copied to the Windows clipboard and inserted and pasted into another supported application (ex. a graphics program, MSPaint, or a word processor);
- The plot can be printed as is, or can be incorporated into a Printing Template which can include project information, company details, and your company logo.
- The plot may be printed to a Post-Script file, and distilled using a distiller tool.

4.4.1 Save as Metafile

When you have any plot window open, you can save the plot as a Windows Metafile (graphics format) by selecting **File** from the main menu and then **Save**. In the **Save File...** dialogue that appears, enter a filename for this file and press **[Save]**. You can now open and manipulate this image using a graphics editor or insert this .WMF file into a report. When using this feature, each plot window must be saved as an individual metafile.



4.4.2 Copy Plot to Clipboard

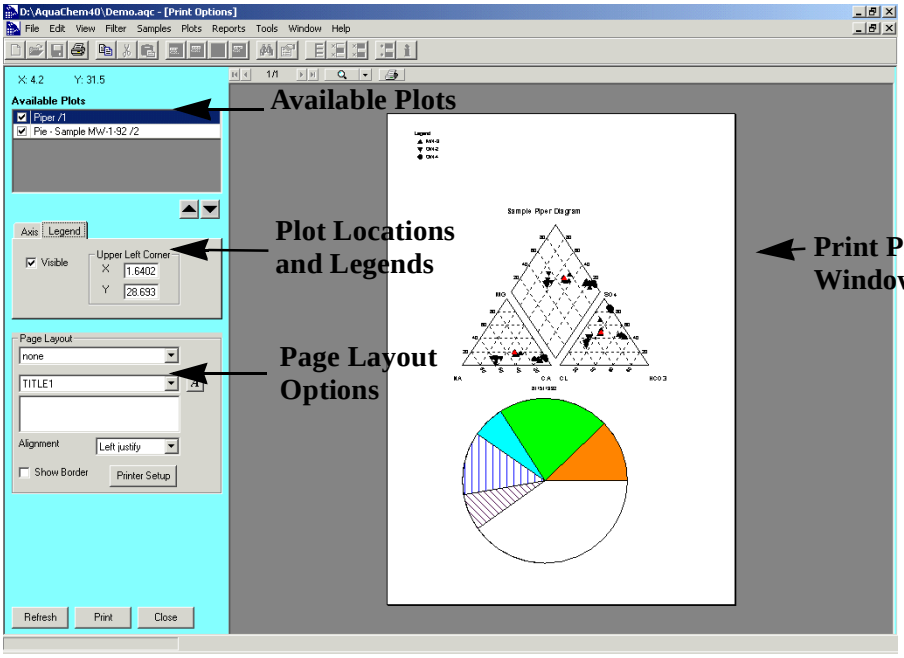
To copy the selected plot to the windows clipboard, select **Edit** from the main menu and then **Copy**. If successful, a confirmation dialogue will appear.

The plot can then pasted directly into another application such as a word processor or a graphics editor.

4.4.3 Printing

To print one or more of the on-screen plots, select **File** from the main menu and then **Print**, while the plots window is active. Alternatively, you can press the  icon from

the AquaChem toolbar. A **Print Options** window will appear, as shown in the figure below:



The **Print Options** window has the following components:

Available Plots: Contains the list the plots which are available for printing

Plot Locations and Legends: Lists the X, Y location of the plot, and the Legend location (if available).

Page Layout Options: Lists the available plot templates, and title and footer entries.

Print Preview Window: Provides a preview of the printed page.

To print one or more plots, you must select the desired plot(s) from the list of the **Available Plots** by placing a check mark in the box beside the appropriate plot. The selected plot(s) will appear in the **Print Preview** window and will be automatically sized and arranged to fit the page.

To select a plot, click once in the box beside the plot name. A check mark will be added to the box and this plot should appear in the Print Preview window. To load additional plot(s), simply click once with your mouse in the box beside the plot name.

To remove a plot from the Print Preview window, simply click once in the box to remove the check mark beside the appropriate plot.

Arranging the Plots

The order of the plots can be easily modified using the arrow buttons below the list of plots. Selected plots can be moved up or down using these buttons. The position of each plot can be modified in the **Axis** tab by entering a new X, Y origin; the size of each plot can be modified by entering a new X, Y length. Or, you can click the **[Auto]** button, and AquaChem will automatically calculate the optimal size and location for the plot. Press the **[Refresh]** button to update the print preview.

Print Preview Window

The Print Preview window provides a “What You See Is What You Get” (WYSIWYG) preview of the printed page. The page magnification value can be adjusted using the magnifying glass above the preview window. This will enlarge or shrink the appearance of the page preview on your screen. The page coordinates (cm) for the mouse pointer location are located in the upper left corner of this window.

Selecting a Print Template

The **Page Layout** frame allows you to select from a list of pre-defined print templates which contain fields for descriptions of the plot(s), the project, client, and company information.

AquaChem includes the following pre-defined print templates:

- US Letter - Portrait
- US Letter - Landscape
- A4 - Portrait
- A4 - Landscape

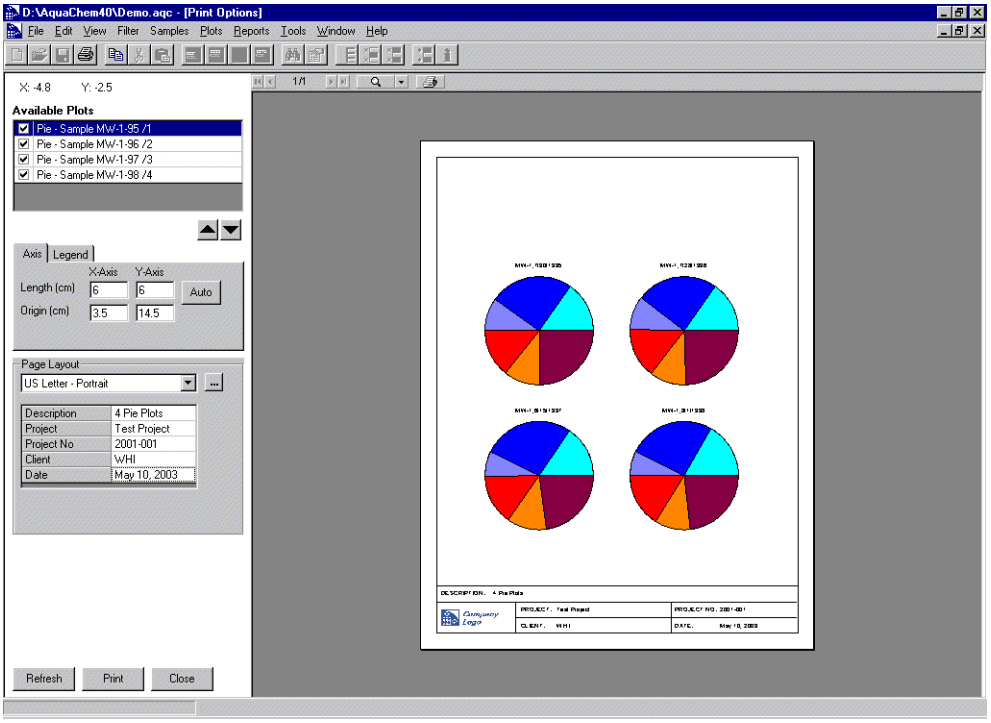
The default template selection is "**None**", meaning no print template is selected. If "**None**" is selected you have the option to enter a two line title at the top of the page plus a footer at the bottom of the page.

If the pre-defined print templates are not satisfactory for your needs, you can easily create your own customized print templates using the **Template Designer** option available in the **File** menu. For a detailed description of this component, please refer to Chapter 3: **Template Designer**

If you select one of the pre-defined print templates, a list of available descriptor fields will appear and the **Print Preview** window will be updated to reflect the layout of the

selected template. Fill in the project specific plot description fields under the **Page Layout** options. Depending on the template, you may enter information for: CLIENT, PROJECT, PROJ #, DATE, DESCRIPTION.

An example of the **Print Preview** window with Fields is shown below:



Once you have entered the descriptive information for the plot, press the **[Refresh]** button to refresh the print preview.

When you are satisfied with the print layout, simply press the **[Print]** button in the lower left corner of the window, or select **File > Print** from the main menu, or press the  icon.

Alternatively, you may select **Edit > Copy** from the main menu, and the plot, along with the print template, can be copied to the clipboard, and pasted into an external application.

To return to the main AquaChem window, press the **[Close]** button.

4.5 Plot Details

This section describes each of the AquaChem plots and the options available for each plot.

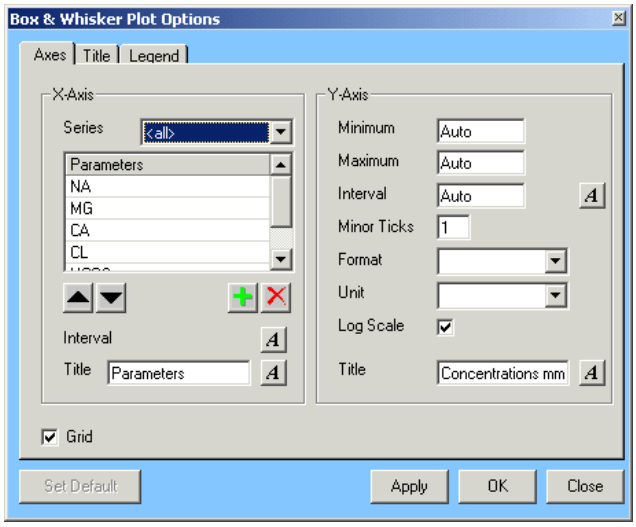
4.5.1 Box and Whisker

The **Box and Whisker** plot displays a statistical summary of any measured database parameter(s).

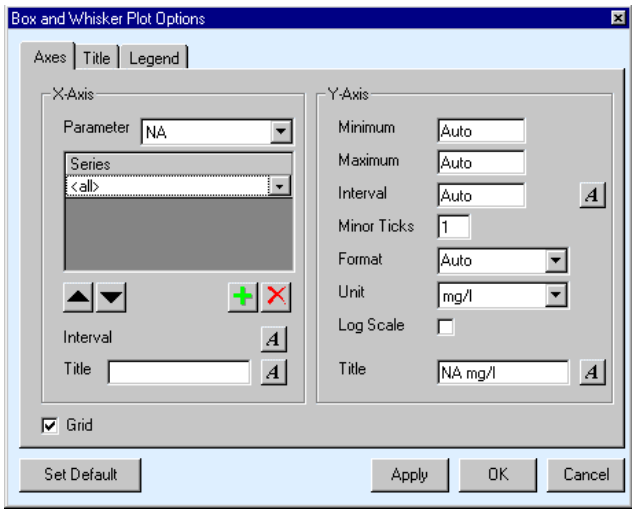
The Box and Whisker plot can be displayed in two forms:

- **Box and Whisker (Multiple Parameters)**
- **Box and Whisker (Multiple Stations)**

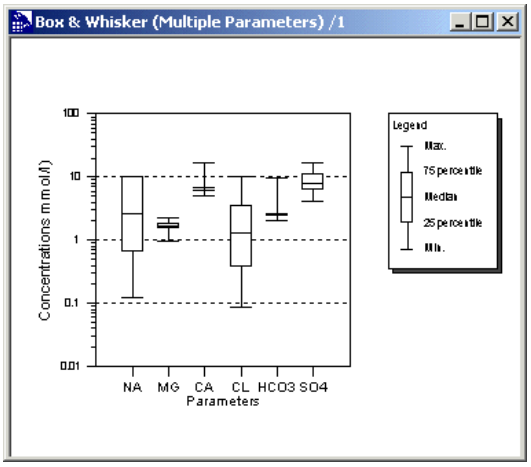
If you select **Box and Whisker (Multiple Parameters)** plot then select ONE station group in the **Series** field, and then specify one or more parameters under the **Parameters** list. If **<all>** is selected, then all samples from the active list will be used. The options for this plot are shown below.



If you select **Box and Whisker (Multiple Stations)** plot then you will see the **Parameters** and **Series** fields become reversed. You need to specify ONE parameter beside the **Parameter** field and then enter one or more station in the **Series** field. The options for this plot are shown below.



An example of the **Box and Whisker (Multiple Parameters)** plot is shown in the figure below.



If you require a logarithmic transformation of the data (e.g. to normalize the data), then select the **Log Scale** option in the plot options dialogue.

There are several derivations of the Box and Whisker plot available. However, the version used in AquaChem does not plot outliers or extreme values as separate points or “dots”. Instead the extreme or outlier values are included in the plot, and may be plotted as the maximum or minimum value, depending on the corresponding value in the database.

As depicted in the **Legend**, there are five components in a **Box and Whisker** plot. From bottom to top they are:

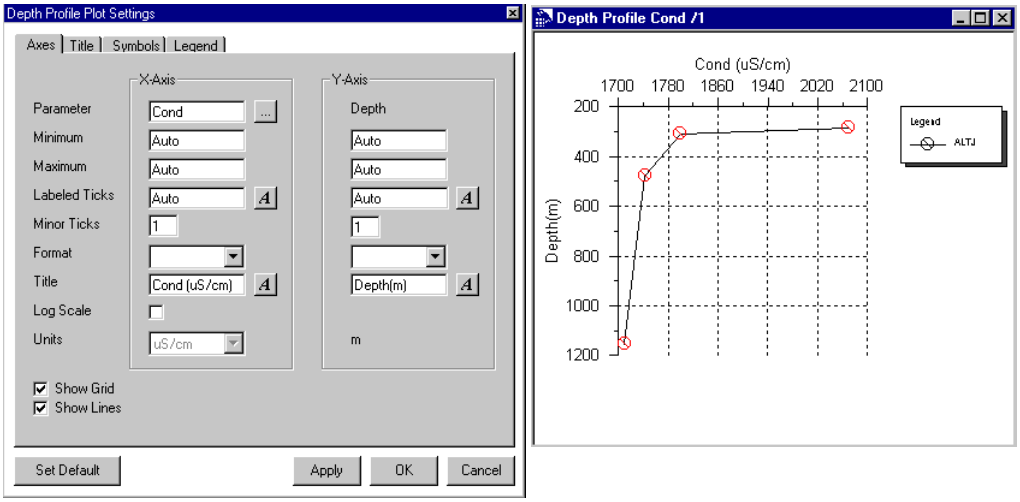
- The minimum (**Min.**);
- Q1: the first (lower) quartile (**25th percentile**): 25% of the data lie below this value;
- Q2: the second quartile (**Median**): 50% of the data lie below this value;
- Q3: the third (upper) quartile (**75th percentile**): 25% of the data lie above this value;
- The maximum (**Max**)

The central box represents the values from the lower to upper quartile (25th to 75th percentile). The middle line represents the median. A vertical line extends from the minimum to the maximum values.

For more details on this plot, please refer to the article: Tukey J.W., 1977: *Exploratory Data Analysis*, Addison-Wesley, Reading, Massachusetts, USA. 1977, pp. 39-43.

4.5.2 Depth Profile

The Depth Profile plot displays the change in a parameter value as sample depth changes. An example of a **Depth Profile** plot and the corresponding **Depth Profile Plot Settings** dialogue is shown in the figure below.

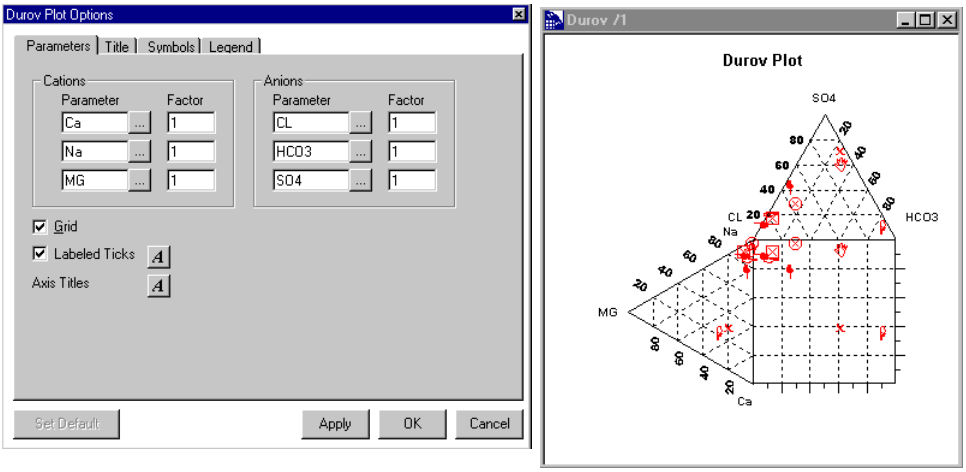


The Depth Profile plot is similar to a borehole log done in the field; the plot displays the change of a measured parameter over a measured sampling depth. In order to create this plot, you must have an entry for the parameter Sample_Depth for one or more samples

in your database. You may then plot the **Depth** (on the Y-Axis) against any measured parameter (on the X-Axis).

4.5.3 Durov Plot

The trilinear Durov plot is based on the percentage of major ion milliequivalents. An example of **Durov** plot and the corresponding **Durov Plot Options** dialogue is shown in the figure below.



In the **Durov Plot Options** dialogue, the **Cations** specify the parameters of the left triangle. Default settings are the major cations **Na**, **Ca**, and **Mg**, however any other parameter can be selected (e.g. gas composition, trace elements etc.). The **Anions** specify the parameters for the upper triangle. Default settings are the major anions **Cl**, **SO4**, and **HCO3**, however any other parameters can be selected.

Data from poorly concentrated parameters can be multiplied by a common factor to prevent data point accumulation on a base line. Type the multiplication **Factor** in the field beside the parameter.

The **Cations** and **Anions** values are plotted on two separate triangular plots and the data points are projected onto a square grid at the base of each triangle. The Durov plot is an alternative to the Piper plot which is described later in this chapter.

Since the data points are projected along the base of the triangle, which lies perpendicular to the third axis in each triangle, information about the concentration of the vertex element (the third element) is lost in the square grid. Changing the orientation of parameters in both triangles may improve your ability to detect distinct groups.

4.5.4 Geothermometer Plot

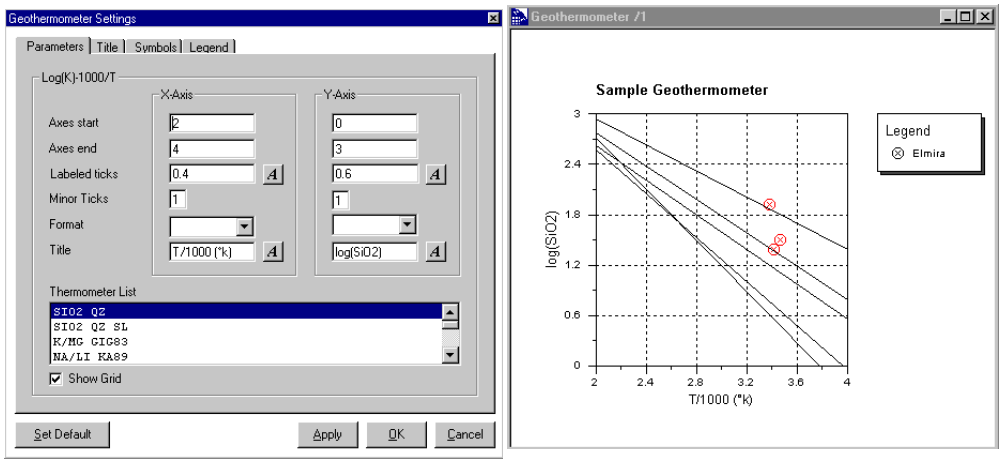
Geothermometer plots can be used to test the quality of geothermometer estimates for a given geological and hydrogeological situation. Different geothermometers can produce very different results when applied to the same water sample(s). Each geothermometer has a set of conditions which must exist for reasonable values to be calculated. For example, if the in-situ temperature was not sufficient to attain rock-water equilibrium, the aquifer composition may be different from the one assumed by the geothermometer. Using conventional geothermometer graphs (log K-1000/T plots), you can check the quality of the calculated temperature if you have precise in-situ temperature measurements. You should collect all analyses from the literature for which in-situ temperatures have been measured. Also note the aquifer lithology of the samples. When you start a geothermal study, search for references to samples which compare closely with the aquifer of the water you are studying, and check which geothermometer gives the most reliable estimates. This thermometer is likely to give the most reliable results for the water you are studying.

Geothermometer plots can be used to:

- Check the applicability of a thermometer on a set of samples.
- Plot the chemistry versus the formation temperature for samples produced from a borehole.
- Search for the geothermometer for which you observe the best fit.
- Develop new chemical thermometers for parameters or parameter ratios which show linear behavior in this plot.

For a list of the available Geothermometers, please see the Thermometers options, in the **File > Database** dialogue.

The Geothermometer plots display commonly used geothermometers. An example of a **Geothermometer** plot and the corresponding **Geothermometer Plot Options** dialogue is shown in the figure below.



The following section describes some of the features and options of the **Geothermometer Plot** that are not covered in the Common Plot Features section.

Geothermometers are generally expressed by the formula:

$$t(K°) = \frac{1000 \cdot a}{b + \log(x)}$$

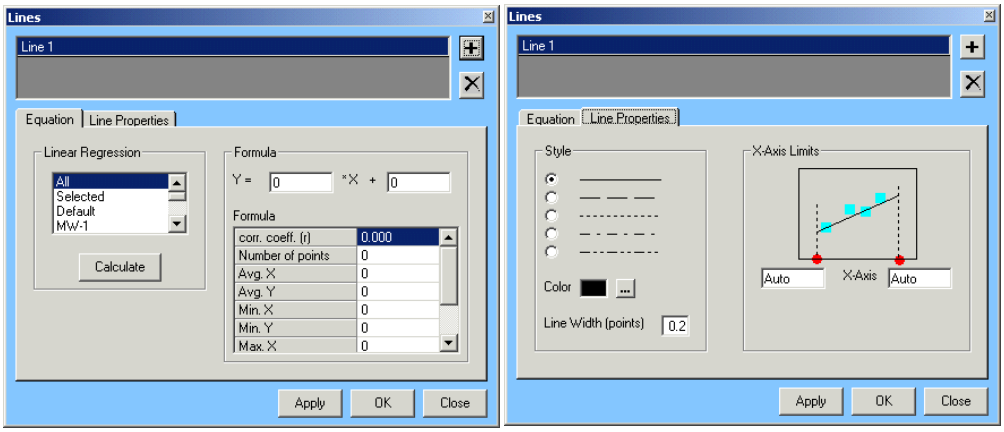
where, x is the SiO_2 concentration or Na/K, etc., *log (x)* values plot on a straight line as a function of 1000/T. The coefficients *a* and *b* are obtained from the linear regression curve.

Log(K)-1000/T

The linear log(K)-1000/T plots can be used for samples from boreholes, where the in-situ temperature is known. In geothermal investigations however, you rarely know the formation temperature and if you do there is no need to apply a geothermometer. If you follow the technique explained above, you will be able to decide which geothermometer to use in other projects with similar water chemistry and aquifer lithology settings. If the geothermometers provided in AquaChem do not meet your needs, you can also develop your own geothermometers and save them for each project (for more details see Thermometers in Chapter 3).

Under the **Symbols** tab, the **[Edit Lines]** button opens the **Lines** dialogue, as shown below. The Lines options allow you to perform a regression analysis on all the data, or on a selected group of data. You can calculate the equation of best fit for the line, and plot the line on the graph. You can also create your own line with your own equation and plot it on the graph as well.

The **Line** dialogue contains two tabs, **Equation** and **Line Properties**.



Equation Tab

The equation of the straight line is displayed under the **Formula** frame. If the equation is calculated by the regression routine rather than entered manually, the **corr. coeff. [r]** is displayed under the **Statistics** frame below the **Formula** frame.

The linear regression analysis can be performed on **All** active samples in the sample list, on **Selected** samples, or on the defined groups of samples.

To calculate and plot a line on the graph:

- Click the + button and **Line 1** will appear in the list of lines (more than one line can be plotted on each graph).
- Choose whether you want to calculate the linear regression using All samples, Selected samples, or a selected group of samples.
- Click the **[Calculate]** button to calculate the equation of the line through the selected data points.
- The resulting formula appears in the **Formula** frame. Descriptive statistics including the regression coefficient for the points selected will appear in the **Statistics** frame.

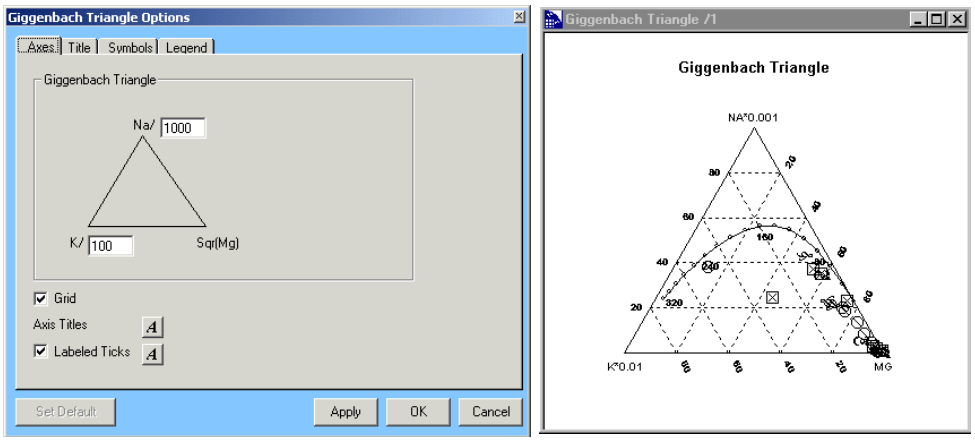
Line Properties Tab

The **Line Properties** tab allows you to select the line type (style), thickness and color as well as the start and end coordinates of the line in the **X-Axis Limits** frame.

For more details on Geothermometers, please refer to the following article:
Kharaka et al. 1989.

4.5.5 Giggenbach Triangle

The Giggenbach Triangle provides a visual aid to determine the water-rock equilibrium. An example of the **Giggenbach Triangle** plot and the corresponding **Giggenbach Triangle Options** dialogue is shown in the figure below.



The Giggenbach Triangle (K-Mg-Na Triangle) representation allows you to verify the extent to which water-rock equilibrium has been attained.

The triangle is comprised of three zones:

- Immature waters (at the base);
- Partially equilibrated waters (in the middle); and
- Fully equilibrated waters (along the upper curve).

Depending on where the composition of a given sample lies within this triangle, you can estimate the extent of rock-water equilibrium. For mature waters falling near the upper curve, you can estimate the temperature as well.

To plot the K-Mg-Na triangle, enter the division factors for Na and K in the text fields provided and press **[OK]**. The default values for the plot are Na/1000 and K/100.

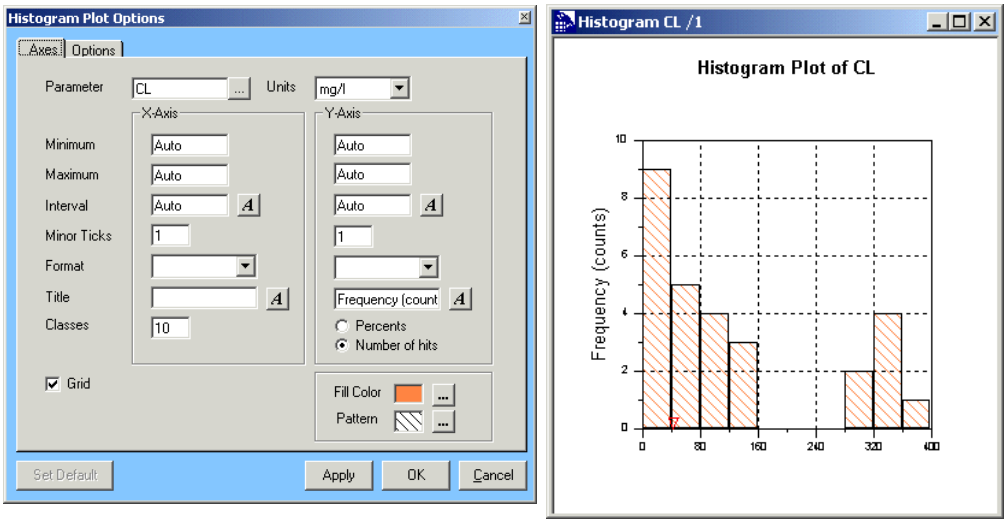
The **Line** options are identical to those for the **Geothermometer** plot; please refer to this section (above) for more details.

For more details on the Giggenbach Triangle, please refer to the following article:

Giggenbach, W.F., 1988. *Geothermal solute equilibria*. Derivation of Na-K-Mg-Ca geoindicators. Geochim Cosmochim. Acta, 52: pp. 2749-2765.

4.5.6 Histogram

Histograms are primarily used to check the population of data within a given range of values. Histograms allow a large number of samples to be represented on just one plot, allowing for quick interpretation. An example of a **Histogram** plot and the corresponding **Histogram Plot Options** dialogue is shown in the figure below.



You can easily identify a single sample in a multi-sample histogram plot by clicking on the sample in the Active Samples List. A red triangle will be displayed on the histogram, indicating the range interval of the selected sample (this is a unique feature of AquaChem and is not normally found in other histogram plotting software). Clicking on a bar on the graph will select all the samples in the Active List which are included within the interval range defined by the histogram bar you selected.

The following section describes some of the features and options of the **Histogram** plot that are not covered in the Common Plot Features section.

The **Parameter** field requires the Internal name of the parameter of interest for the Frequency Histogram. The parameter of interest can be typed in directly if you know the Internal name, or you can select another parameter from the measured parameters list. This field can also handle parameter ratios, sums, or differences (e.g. Na/Cl, Ca+Mg, Cl-SO4). Enter these parameter combinations into the parameter field manually.

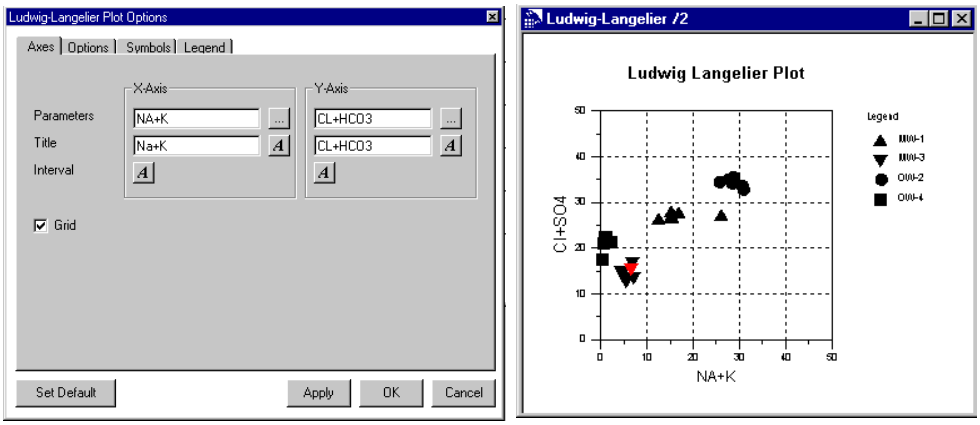
The **Classes** field defines the number of data classes (or intervals) into which the range of parameter values will be subdivided. Each data class will be represented by a single bar on the histogram. Type the number of classes (bars in the histogram) in the provided field.

The number of samples within each data class is referred to as the frequency of occurrences. This can be expressed as either a percentage of the total number of samples (**Percents**), or as the number of samples within each data class (**Number of hits**).

Finally, the color and pattern of the bars in the graph can be modified using the options beside **Color** and **Pattern**. Simply press the ... button to access the various options.

4.5.7 Ludwig-Langelier Plot

The Ludwig-Langelier plot allows you to quickly see patterns and correlations between the major cations and anions for multiple samples. An example of the **Ludwig-Langelier** plot and the corresponding **Ludwig-Langelier Plot Options** dialogue is shown in the figure below.



The Ludwig-Langelier square plot is similar to the projection areas of the Piper and Durov plots. By convention, the sums of selected cations are plotted on the **X-Axis** and the sums of selected anions are plotted on the **Y-Axis**. Each axis ranges from 0 to 50 meq%. Sample points are calculated as follows:

$$\Sigma anions = Cl + SO4 + HCO3$$

$$\Sigma cations = Ca + Mg + Na + K$$

$$\%\, Na = 50\, \frac{Na}{\Sigma cat}$$

$$\%Cl = 0\frac{Cl}{\Sigma an}$$

Suitable groupings of cations and anions are selected and plotted as percentages. Generally, this type of graph is used to plot %Na+%K against %HCO3+%SO4. In this plot, %Ca+%Mg and %Cl are also fixed:

%Ca+%Mg =50 - (%Na+%K)
%Cl =50 - (%HCO3 +%SO4)

Changing the groupings of anions and cations often improves the identification of water with a particular chemical type. For instance:

- %Na+%K+%Mg against %HCO3: cold, low salinity calcium bicarbonate waters (limestones).
- %Na+%K+%Ca against %HCO3: cold, low salinity magnesium bicarbonate waters (mafic and ultramafic rocks).
- %Na+%K+%Mg against %HCO3+%Cl: cold, calcium sulfate waters (gypsum and/or anhydrite).

All major elements can be displayed in one plot with the Ludwig-Langelier plot, however like the Piper and Durov plots, the plot displays relative ratios rather than absolute concentrations.

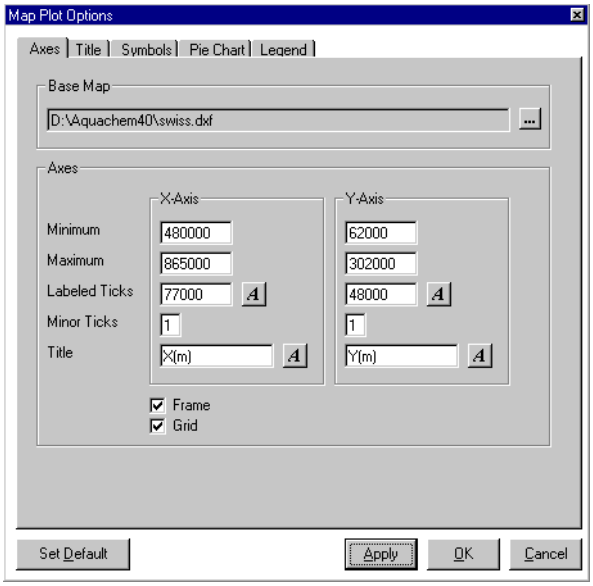
4.5.8 Map Plot

The Map Plot reads the X, Y coordinates for the station location, and displays this on a blank grid or on a site map of your site. The Map plot can import and overlay an AutoCAD .DXF file as a basemap of the site or study region defining the major physical and geographical boundaries and geological characteristics.

The Map plots can be used to simply display the station locations throughout the study region, or you can use the Map plot to interpret spatial trends in the physical or chemical characteristics of each sample using proportional symbol sizes, or by plotting **Pie**, **Radial** or **Stiff** graphs at each sample location.

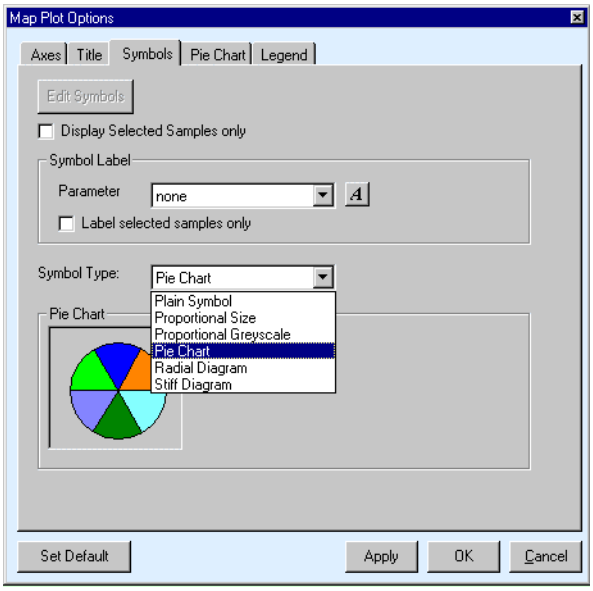
NOTE: You must have at least one station in your database with X and Y co-ordinates in order to create a Map plot.

When you choose a **Map** as the plot type, the following **Map Plot Options** dialogue will appear:



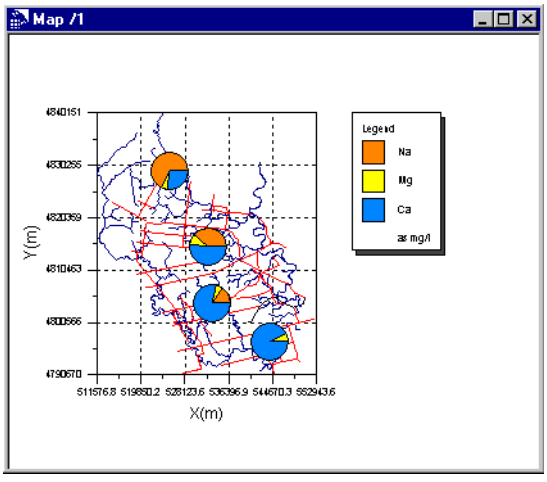
Click the **...** button beside the **Base Map** field to locate and select the **.DXF** file to use as a basemap. AquaChem supports AutoCAD version 14 .DXF file formats. Please note that this option is intended for relatively small and simple map files (.DXF site maps larger than 1 Mb may take a long time to load, or may not load at all). If the .DXF file does not load, try to remove any unnecessary detail and objects from the map, and import a scaled-down, simplified version of your site map.

The start and end coordinates (**Minimum** and **Maximum**) of the base map are automatically displayed after you have imported the .DXF base map file; the coordinates are read from the .DXF file. You may edit the **Minimum** and **Maximum** to zoom in on part of your base map. Since each station in the database is referenced with X and Y coordinates, the range specified in the Axes frame will determine which corresponding stations will be plotted on the graph. If the coordinate locations of the station does not correspond to the coordinate dimensions of the basemap, none of the samples associated with these stations will appear on the Map plot. The **Symbols** tab in the **Map Plot Options** dialogue allows you to choose from a selection of six different symbol types for each sample location:



- Plain Symbol
- Proportional Size
- Proportional Greyscale
- Pie Chart
- Radial Diagram
- Stiff Diagram

An example of a **Map Plot** with **Pie** charts as sample symbols is shown below.



The following section describes the various symbol types and the display options available for plotting each symbol on the site map.

Map - Plain Symbol

The Plain Symbol type will plot the symbol shapes, sizes and colors as they are defined for each sample group. Press the **[Edit Symbols]** button to access the **Define Symbol or Line** dialogue for viewing or modifying the symbol settings for the database.

Map - Proportional Size Symbols

The Proportional Size symbol type will plot the defined symbols at each sample location with a symbol size determined by the value of a selected parameter. By default, AquaChem selects **Na** as the proportional parameter. The sample values for the proportional parameter will be used to determine the radius of the symbol at each sample location (e.g.samples containing higher values of the proportional parameter will have a larger symbol radius).

To change the proportional parameter, simply type in the Internal name of the desired parameter in the **Parameter** field, or click the  button and select another parameter from the list.

The **Radius** field is used to set the minimum and maximum symbol radius (in points). The minimum symbol radius corresponds to the **Lower Limit** value of the proportional parameter, while the maximum radius corresponds to the **Upper Limit** value. Use a non-zero minimum radius to plot symbols at sample locations containing very low values of the proportional parameter. The symbol radius at each sample location is determined using a linear interpolation between the **Upper Limit** value and the **Lower Limit** value.

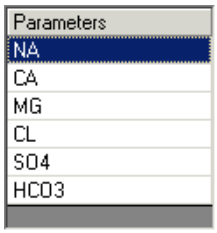
Map - Proportional Greyscale

This symbol type will display a Greyscale symbol at each sample location, with the scale determined by the value of a selected parameter. By default, AquaChem selects **Na** as the proportional parameter. The sample values for the proportional parameter will be used to determine the greyscale color of the symbol at each sample location (e.g. samples containing higher values of the proportional parameter will have a darker greyscale). To change the proportional parameter, simply type in the Internal name of the desired parameter in the **Parameter** field, or click the  button and select another parameter from the parameters list.

Sample with values less than the Lower Limit value are assigned a white symbol color, while points with values equal to or greater than the Upper Limit value are assigned a black color fill.

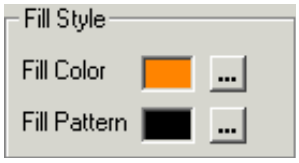
Map - Pie Chart

This symbol type will display a Pie chart of the selected parameters at each sample location. To view or modify the pie chart display settings, press the **[Edit]** button, or click the **Pie Chart** tab on the **Map Plot Options** dialogue.

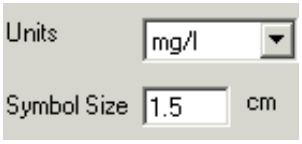


The parameters plotted on the pie charts are shown in the **Parameters** list box on the left-hand side of the dialogue.

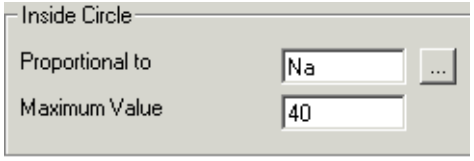
The parameters are plotted in counter-clockwise order, where the first parameter in the list starts at the three o'clock position in the circle. The order of the parameters in the list box can be modified by selecting the parameter and using the  or  buttons to move the position of the selected parameter. Additional parameters can be added to the list by pressing the  button and choosing a parameter from the available list.



The **Fill Style** (**Fill Color** and **Fill Pattern**) for each parameter can be modified by clicking on the target parameter, then choosing a new Color or the Pattern by clicking on  button beside **Fill Color** and **Fill Pattern** fields.



The **Units** field contains a selection of available concentration units for the selected pie chart parameters which can be selected by clicking on the  button. The **Symbol Size** field contains the setting for the size of the pie charts plotted at each sample location.



The **Inside Circle** option plots an open circle at the centre of the pie chart, where the radius of the open circle is **Proportional to** the concentration of the proportional parameter. The maximum radius of the inside circle is one-half of the radius of the pie chart circle. The samples containing a Proportional parameter concentration equal or greater than the **Maximum Value** will have an inside circle with the maximum radius. The inside circles for samples with Proportional parameter concentrations less than the Maximum Value will have a proportionally smaller radius.

Under the **Legend** tab of the **Map Plot Options** dialogue, you may adjust the **Legend Size** for the pie chart as it will appear on the map plot.

Map - Radial Diagram

This plot will display a Radial Diagram of the selected parameters at each sample location. If the **Radial Diagram** is selected from **Symbol Type** field, a schematic drawing of a sample radial plot is displayed in the lower left corner of the **Map Plot Options** dialogue. To view or modify the radial plot display settings, press the **[Edit]** button, or click on **Radial Diagram** tab on the **Map Plot Options** dialogue.

The parameters plotted on the Radial diagram are shown in the **Parameters** list on left side of the dialogue. The parameters are plotted in counter-clockwise order, where the first parameter in the list starts at the three o'clock axis position.

The order of the parameters in the list box can be modified by selecting the parameter and using the  or  buttons to move the position of the selected parameter. Additional parameters can be added to the list by pressing the  button and choosing a parameter from the available list.

The **Fill Style** (**Fill Color** and **Fill Pattern**) for each parameter can be modified by clicking on the target parameter, then choosing a new Color or the Pattern by clicking on  button beside **Fill Color** and **Fill Pattern** fields.

In the **Axes** field, the **Minimum** and **Maximum** axes values will apply for all Radial diagram symbols plotted on the map. The minimum axes value will reflect the parameter value at the centre of the radial diagram, while the maximum axes value will represent the uniform maximum parameter value at the end of each axis. The minimum value is zero by default, and the maximum value is uniform for each axis of the radial diagram.

The **Unit** field contains a selection of available concentration units for the selected parameters.

The **Symbol Size** field contains the setting for the size of the Radial diagrams plotted at each sample location.

Under the **Legend** tab of the **Map Plot Options** dialogue, the **Legend Size** field contains the setting for the size of the radial plot legend as it will appear on the Map plot.

Map - Stiff Diagram

This plot will display a Stiff diagram of the selected parameters at each sample location. If the **Stiff Diagram** is selected from **Symbol Type** field, a schematic drawing of a sample Stiff diagram is displayed in the lower -left corner of the **Map Plot Options**

dialogue. To view or modify the Stiff diagram display settings, press the **[Edit]** button or click on **Stiff Diagram** tab on the **Map Plot Options** dialogue.

The parameters plotted on the Stiff diagrams are shown in the Parameter list labelled **Cations** and **Anions**. By default, the six major ions are included in the Stiff diagram. The parameters at the top of the list will appear on the top of the Stiff diagram.

The order of the parameters in the list box can be modified by selecting the parameter and using the  or  buttons to move the position of the selected parameter. Additional parameters can be added to the list by pressing the  button and choosing a parameter from the available list. Parameter combinations can also be used (e.g. Na+K).

The **Fill Style** (**Fill Color** and **Fill Pattern**) for each parameter can be modified by clicking on the target parameter, then choosing a new Color or the Pattern by clicking on  button beside **Fill Color** and **Fill Pattern** fields.

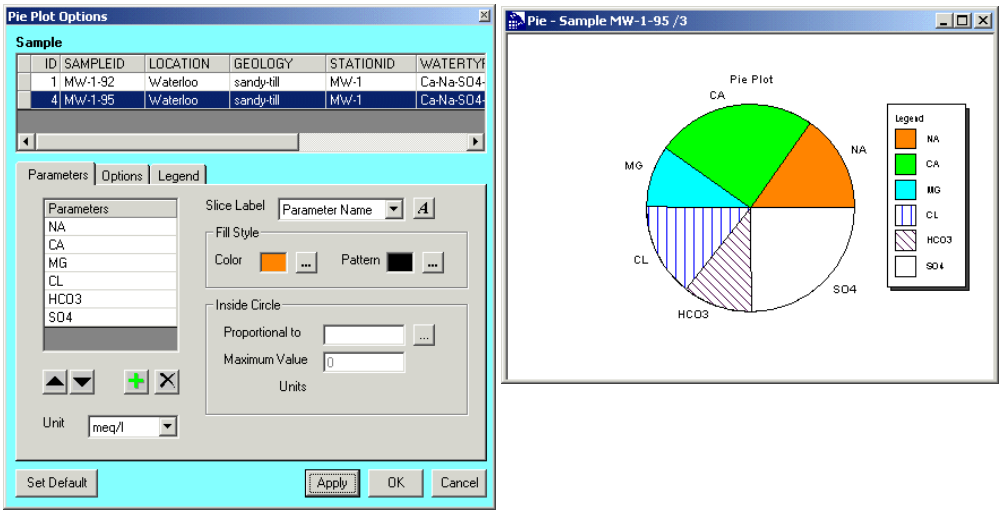
The **Maximum Concentration** values will represent the uniform maximum value for each parameter. This value cannot vary for each axis of the Stiff diagram. The minimum axes value is always zero.

The **Symbol Size** field contains the setting for the size of the Stiff diagrams plotted at each sample location.

Under the **Legend** tab, the **Legend Size** field contains the setting for the size of the Stiff plot legend as it will appear on the Map plot.

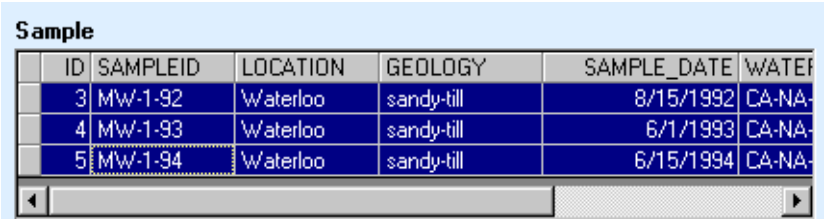
4.5.9 Pie Plot

The Pie plot is a simple way of showing parameter portions in a sample. An example of the **Pie** plot and the corresponding **Pie Plot Options** dialogue is shown in the figure below.



When you choose the **Pie** chart, a plot will be created for every sample selected in the active sample list. Before using this option, ensure that only the samples you want to plot are selected.

At the top of the **Pie Plot Options** dialogue, there is a **Sample** field which identifies the active sample(s) associated with the plot options dialogue. If you have created several Pie charts, you can use the **Sample** field to select and modify the settings for each pie plot individually, or all at once as shown below.



To make changes to multiple plots simultaneously, simply select all of the samples in the list above (using your mouse), make the required plot changes then click **[Apply]**. This is useful for normalizing the axes scales, units, and general formats for each of the open Pie charts. The changes applies to most of the graph settings that affect the appearance of the Pie chart, with the exception of the plot title. If just one sample is highlighted and selected in this dialogue, then the changes will only be applied to this plotted sample.

The **Parameters** list contains the parameters that will be plotted on the Pie chart. Existing parameters can be changed by selecting on the parameter, and then typing in the name of the new parameter in the same field. New parameters can be added to the

list by clicking the  button and selecting a parameter from the available list. The new parameter will then be added to the bottom of the list. Parameters can be removed from the list by selecting the parameter and clicking the  button. The order of the parameters in the list can be adjusted using the up and down buttons.

The **Slice Label** options will apply a label to each slice of the pie chart. You can choose from **Parameter Name**, **Concentration**, **Percentages**, or **None** for no label.

The **Fill Style** allows you to edit the appearance of each pie slice in the plot. Select a parameter from the Parameters list, then select the **Pattern** and the **Color** you wish to assign to that slice of the pie chart. Repeat for the other parameters in the list.

The **Inside Circle** is used to represent the concentration of a single parameter (or combination of parameters) that is not included in the Pie Chart parameters. You can specify any chemical or physical parameter that reveals the most comprehensive information about the sample. For example, you may want to display the CO2 or SiO2 concentration for the selected sample. Type a valid parameter in the **Proportional to** field to create an inside circle on your pie chart. Type a **Maximum Value** in the next field below (or use the default value). If several pie charts are created, it is recommended that you choose 3 to 4 times the average value of the inside parameter as the maximum value. All values that are greater than or equal to the maximum value are displayed with the maximum diameter. The inside circle will have a radius (r) between zero and the specified maximum radius (R).

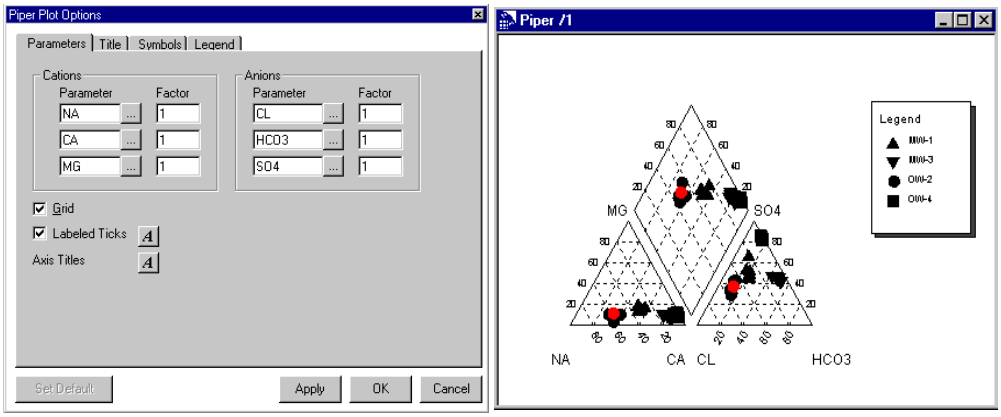
R= Maximum radius for the internal circle
Value = value for this sample for the selected parameter.
Maximum Value: Maximum value above which, the full internal circle is drawn.

Inside Radius = (Value / Maximum Value) * (πR/2)

The Pie charts will be titled automatically using the parameters defined in the **Preferences** section. To enter a new plot title, simply delete the Title and enter the new text. To change the automatic title settings, see the **File > Preferences** section in Chapter 3 of this manual.

4.5.10 Piper Plot

The Piper plot is useful for showing multiple samples and trends in major ions. An example of the **Piper** plot and the corresponding **Piper Plot Options** dialogue is shown in the figure below.



In Piper plots, major ions are plotted as cation and anion percentages of milliequivalents in two base triangles. The total cations in meq/l, and the total anions in meq/l, are set equal to 100%. The data points in the two triangles are then projected onto the diamond grid. The projection reveals certain useful properties of the total ion relationships. Every sample is represented by three data points; one in each triangle and one in the diamond grid.

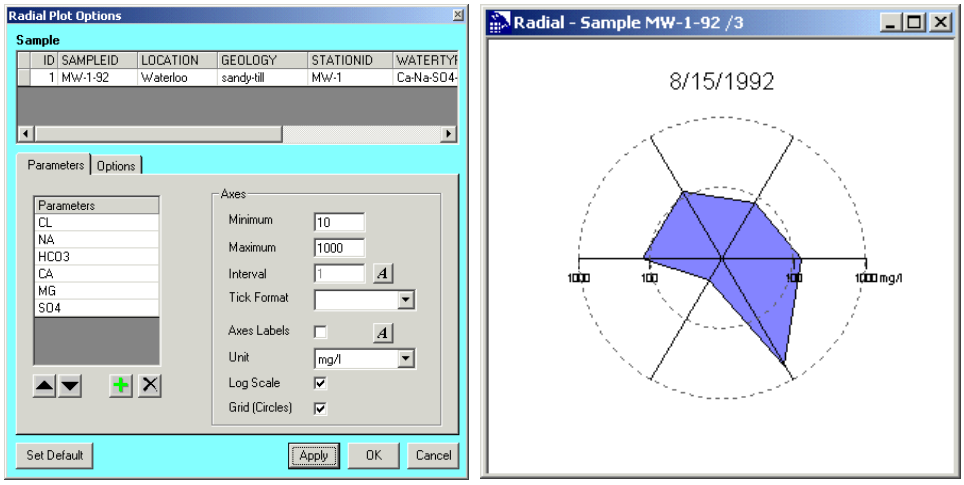
The Piper plot allows comparisons between a large number of samples. Like all trilinear plots, it does not portray absolute ion concentrations. The main purpose of Piper plots is to show clustering of samples.

The default parameter settings include the major cations (Na, Ca, and Mg) against the major anions (Cl, SO4 and HCO3); however, any other parameters, or combination of parameters, can be easily selected (e.g. gas composition, trace elements etc.)

The parameters can be modified by typing the Internal name of the parameters in the appropriate fields, or pressing the ... button and selecting another parameter from the available list. You may also multiply or divide the parameter concentrations by a factor if you need to compare elements which are systematically very different in concentration (e.g. comparing a trace element together with major ions). Finally, you may also enter parameter operators and functions (e.g. Na+K or Na/Cl); to do this, simply enter Na+K (for example) in the parameter field manually, and press **[Apply]**. However multiple parameters (e.g. Na, Cl) are not accepted.

4.5.11 Radial Plot

The Radial plot is used to compare multiple parameter values for a single sample and to compare the ratios of these values for many different samples. An example of the **Radial** plot and the corresponding **Radial Plot Options** dialogue is shown in the figure below.



Radial plots can be used to evaluate the change in water quality at a single location over a period of time, or they can be used to evaluate the change in water quality as the water passes through different geologic formations or different subsurface conditions. A plot will be created for every selected sample in the Active Samples List. Before using this option, ensure that only the samples you want to plot are selected.

The **Sample** field identifies the active sample(s) associated with the plot options dialogue. If you have several Radial plots open, you can use the **Sample** field to select and modify the settings for each one.

To make changes to multiple plots simultaneously, simply select all of the samples in the list above (using your mouse), make the required plot changes, then click **[Apply]**. This is useful for normalizing the axes scales, units, and general formats for each of the open Radial plots. The changes applies to most of the graph settings that affect the appearance of the Radial plot, with the exception of the plot title. If just one sample is highlighted and selected in this dialogue, then the plot options changes will only be applied to this plotted sample.

The **Parameters** list contains the parameters that will be plotted on the Radial plot. A Radial plot requires a minimum of three parameters. Existing parameters can be changed by selecting the parameter, and then typing in the name of the new parameter in the same field. New parameters can be added to the list by clicking the button

and selecting a parameter from the available list. The new parameter will then be added to the bottom of the list. Parameters can be removed from the list by selecting the parameter and clicking the button. The order of the parameters in the list can be modified by selecting the parameter and using the or buttons to move the position of the selected parameter.

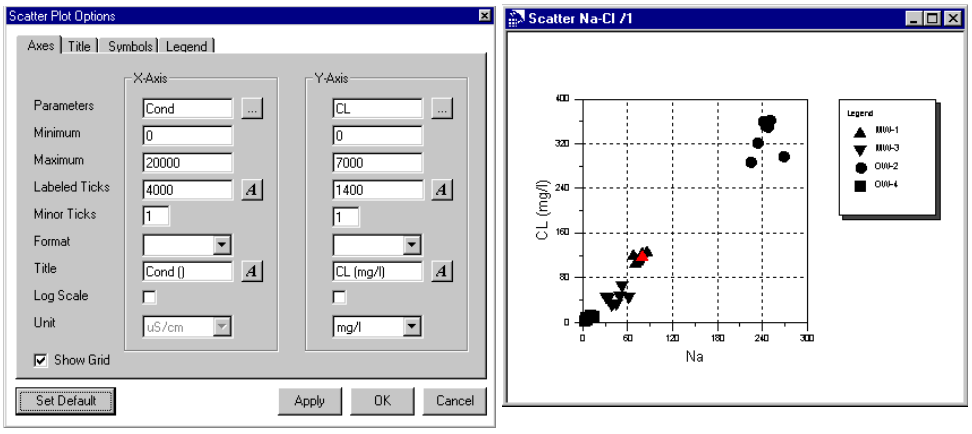
The **Log Scale** check box allows you to switch all of the axes on the radial plot to a log scale. This is often used when the parameters that are plotted range through several orders of magnitude (e.g. when plotting major and minor or trace elements).

Under the **Options** tab, the **Fill Style** will allow you to edit the appearance of the plot. The **Color** and **Pattern** in the **Fill Style** can be modified by clicking on the button.

The Radial charts will be titled automatically based on the parameters defined in the **Preferences** section. To enter a new plot title, simply delete the Title and enter a new text. To change the automatic title settings, see the **File > Preferences** section in Chapter 3 of this manual.

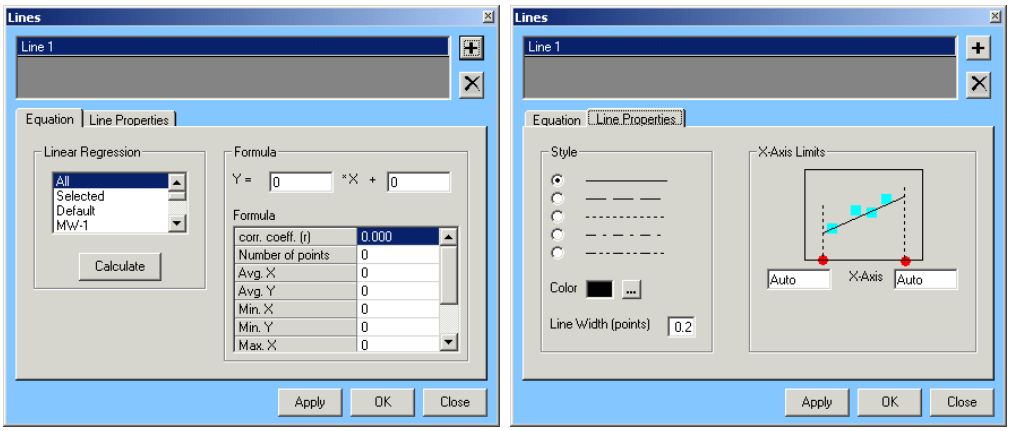
4.5.12 Scatter Plot

X-Y Scatter plots are the most simple approach to interpreting hydrochemical data. Multiple plots of single ion relationships and parameters that show significant correlations can be easily created and regression analyses can be quickly performed to obtain average molal ratios for all data or for selected groups of data. An example of the **Scatter** plot and the corresponding **Scatter Plot Options** dialogue is shown in the figure below.



In the **Axes** tab, the **Log Scale** check box allows you to change the scale of the X and Y axis to log scale. This is often used when you have parameter values that range through several orders of magnitude.

Under the **Symbols** tab, the **[Edit Lines]** button opens the **Lines** dialogue, as shown below:



The **Lines** options allow you to perform a regression analysis on all the data, or on a selected group of data. You can calculate the equation of best fit for the line, and plot the line on the graph. You can also create your own line with your own equation and plot it on the graph as well.

Equation Tab

Under the **Equation** tab the equation of the straight line is displayed. If the equation is calculated by the regression routine rather than entered manually, the **corr. coeff. [r]** is displayed in the **Formula** frame. The linear regression analysis can be performed on All active samples in the sample list, on Selected samples, or on the defined groups of samples.

To calculate and plot a line on the graph:

- Click the + button and **Line1** will appear in the list of lines (more than one line can be plotted on each graph).
- Choose whether you want to calculate the linear regression using **All** samples, **Selected** samples, or a selected group of samples.
- Click the **[Calculate]** button to calculate the equation of the line through the selected data points.

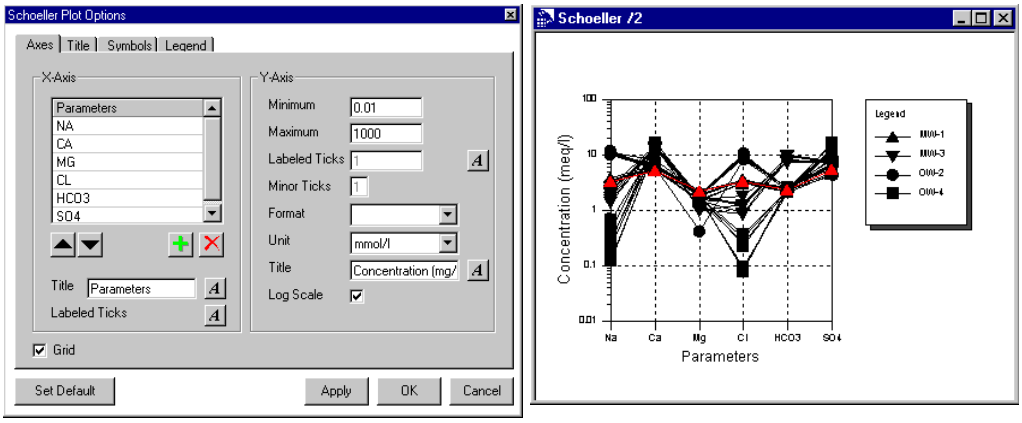
- The resulting formula appears in the **Formula** frame. Descriptive Statistics including the regression coefficient for the points selected will appear in the **Statistics** frame below the equation.

Line Properties Tab

The Line Properties tab allows you to select the line type, thickness and color as well as the start and end coordinates of the line in the **X-Axis** Limits frame.

4.5.13 Schoeller Plot

Schoeller (1962) developed semi-logarithmic plots to represent major ion analyses in milliequivalents per liter and to demonstrate different hydrochemical water types on the same plot. The number of analyses that can be illustrated at one time is limited because of the lines. The plot has the advantage that, unlike trilinear plots, actual parameter concentrations are displayed. An example of the **Schoeller** plot and the corresponding **Schoeller Plot Options** is shown in the figure below.

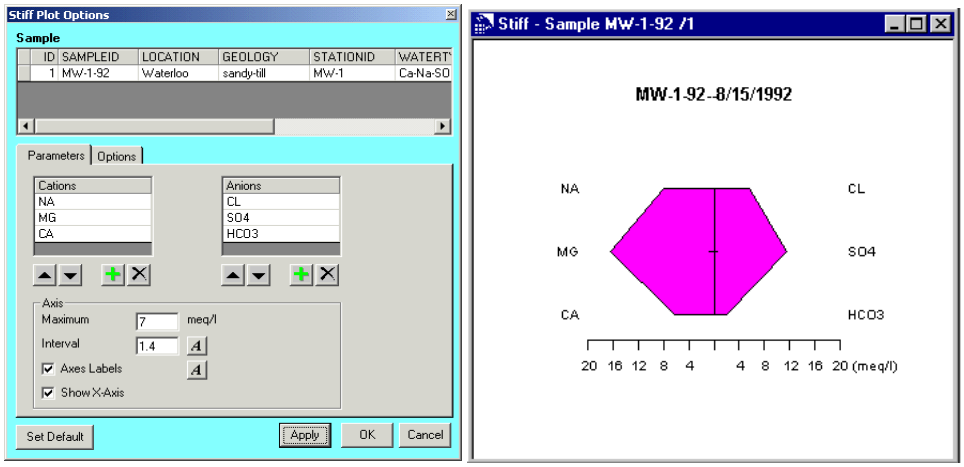


The **Parameters** list defines the parameters that will be plotted on the X-axis of the Schoeller plot. New parameters can be added to the list by clicking the button and selecting a parameter from the list of available parameters. The new parameter will then be added to the bottom of the list. Parameters can be removed from the list by selecting the parameter and clicking the button. The order of the parameters in the list can be modified by selecting the parameter and using the or buttons to move the position of the selected parameter. Parameters can include ratios, sums, or differences (Na/Cl, Ca+Mg, Cl-SO4). Simply manually enter these operators in the parameter field.

4.5.14 Stiff Plot

The Stiff plot belongs to the group of pattern plots (see Hem 1985, p. 175). It is constructed by plotting the milliequivalents per liter of three or more anions and three or more cations. Stiff plots can be used to evaluate the change in water quality at a single location over a period of time, or they can be used to evaluate the change in water quality as the water passes through different geologic formations or different subsurface conditions.

An example of the **Stiff** plot and the corresponding **Stiff Plot Options** dialogue is shown in the figure below.



A Stiff plot will be created for every selected sample in the active list. Before using this option, ensure that only the samples you want to plot are selected. The following section describes some of the features and options of the Stiff plot that are not covered in the Common Plot Features section.

The **Sample** field identifies the active sample(s) associated with the plot options dialogue. If you have several Stiff plots open, you can use the **Sample** field to select and modify the settings for each one.

To make changes to multiple plots simultaneously, simply select all of the samples in the list above, (using your mouse), make the required plot changes, then click **[Apply]**. This is useful for normalizing the axes scales, units, and general formats in each of the open Stiff plots. The changes applies to most of the graph settings that affect the appearance of the Stiff plot, with the exception of the plot title. If just one sample is highlighted and selected in this dialogue, then the plot options changes will only be applied to this plotted sample.

The **Parameters** list contains the parameters that will be plotted on the Stiff plot. Existing parameters can be changed by selecting the parameter, and then typing in the name of the new parameter in the same field.

New parameters can be added to the list by clicking the button and selecting a parameter from the list of available parameters. The new parameter will then be added to the bottom of the list. Parameters can be removed from the list by selecting the parameter and clicking the button. The order of the parameters in the list can be modified by selecting the parameter and using the or buttons to move the position of the selected parameter.

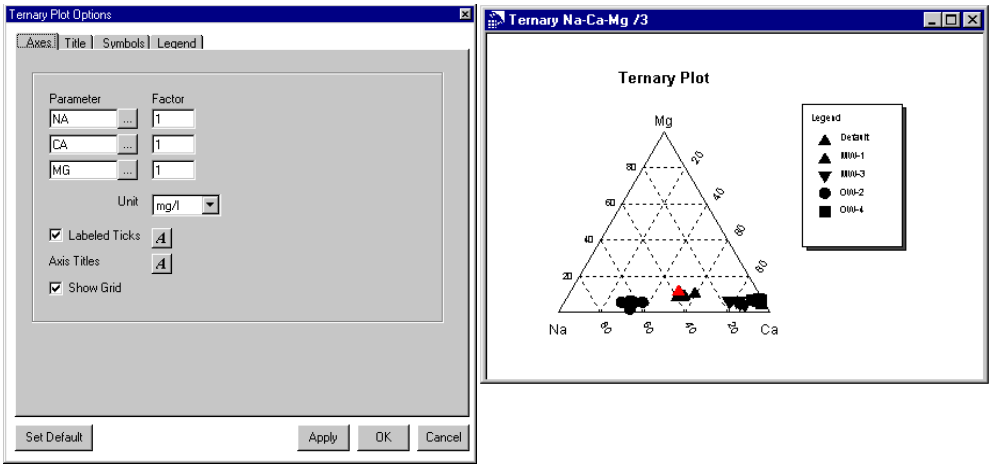
NOTE: The Stiff plot requires an equal number of cations and anions (i.e. typically three cations and three anions).

Under the **Options** tab, the **Fill Style** will allow you to edit the appearance of each plot. The fill **Pattern** and the **Color** options can be accesses by clicking on the button.

The Stiff plots will be titled automatically using the parameters defined in the **Preferences** section. To enter a new plot title, simply delete the Title and enter new text. To change the automatic title settings, see the **File > Preferences** section in Chapter 3 of this manual.

4.5.15 Ternary Plot

Ternary plots are used to determine the relationship between the concentrations of three different parameters in multiple samples. An example of the **Ternary** plot and the corresponding **Ternary Plot Options** dialogue is shown in the figure below.



Like the **Piper** and **Durov** plots, the Ternary plot displays relative concentrations of each parameter with respect to the sum of the concentrations of each parameter. Each vertex of the Ternary plot represents a relative concentration of 100% for the parameter at the respective vertex, while the base represents a relative concentration of 0% for the parameter plotted at the opposite vertex.

The parameters can be modified by typing the Internal name of the parameters in the appropriate fields, or pressing the ... button, and selecting another parameter from the dialogue that appears.

You may also multiply the parameter concentrations by a factor if you need to compare elements which are systematically very different in concentration (e.g. comparing a trace element together with major ions). You may also enter parameter operators and functions (e.g. Na+K or Na/Cl); to do this, simply enter Na+K in the parameter field and press **[Apply]**. However multiple parameters (e.g. Na,Cl) are not accepted.

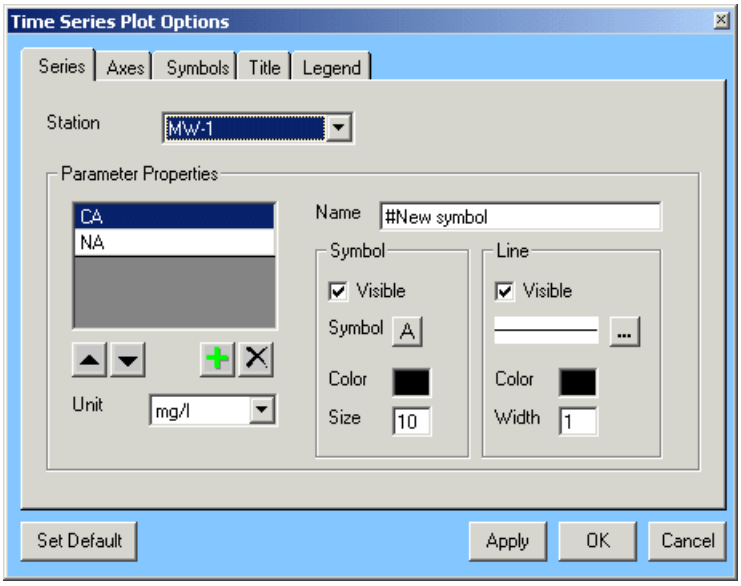
4.5.16 Time Series Plot

The Time Series plot shows the evolution of a chemical or physical parameter for a given sampling point as a function of time. This plot is a standard technique for interpreting hydrochemical and hydrogeological processes in natural waters.

AquaChem allows you to create two types of Time Series plots:

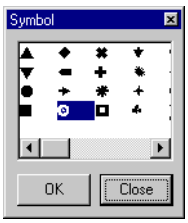
- **Time Series (Multiple Parameters)** for one sampling station; OR
- **Time Series (Multiple Stations)** for one parameter

If the **Time Series (Multiple Parameters)** is selected, then the following options dialogue will appear:



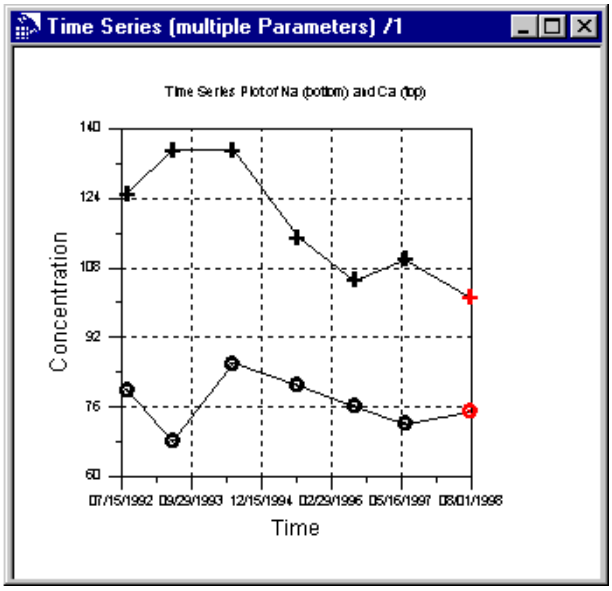
Beside the **Station** field, you must choose a single station using the combo box. Then under the **Parameters Properties** frame below, you may choose the parameter(s) that you want plotted.

Use the  and  buttons to add or remove parameters, and the up  or down  buttons to change the order of the parameters.

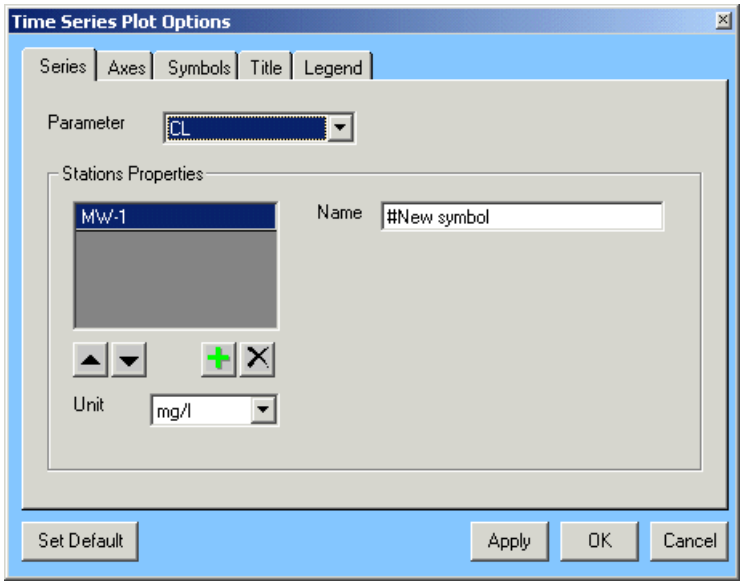


After the parameters are added, you need to specify the corresponding symbols, and symbol names, in the options beside the **Parameter Properties**. To do so, simply select the parameter, and type in a **Name** for the symbol. Then under the **Symbol** frame, you can define the symbol properties (such as **Symbol** type, **Color** and **Size**) in the options below. Press the symbol button beside the Symbol label, and a mini dialog will appear showing the available symbols (as shown to the right). Select a symbol character from here, then click **[OK].**

Under the **Line** frame, you can specify the Line style using  , **Color** and **Width**, and **Visible** to hide or show the line. An example of the **Time Series (Multiple Parameters)** plot is shown in the figure below.



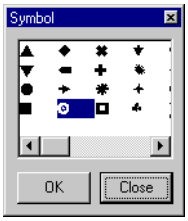
If the **Time Series (Multiple Stations)** is selected, then the following options dialogue will appear.



You must choose a single **Parameter** from the combo box at the top of the options dialogue; then under the **Stations Properties** frame below, you may choose the Stations group(s) that you want plotted. Use the  and  buttons to add and remove stations fields, and choose the stations from the combo box in each field.

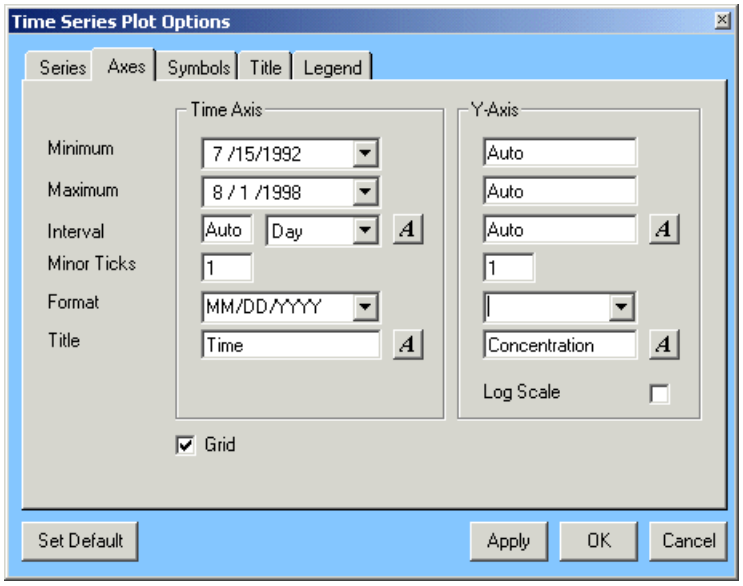
Use the up or down buttons to change the order of the stations.

After the stations are added, you need to specify the corresponding symbols, and symbol names, in the options beside the **Station Properties**. To do so, simply select the station, and type in a **Name** for the symbol. Then under the **Symbol** frame, you can define the symbol properties (such as **Symbol** type, **Color** and **Size**) in the options below. Press the symbol button beside the Symbol label, and a mini dialog will appear showing the available symbols (as shown to the right). Select a symbol character from here, then click **[OK].**



Note that the Time Series plot is limited to one label for the **Y-axis**. As such, it is recommended that you select multiple parameters which have the same measured units (i.e. Do not plot Na and pH on the same time series plot; separate these into two separate time series plots). Future versions of AquaChem will allow you to plot multiple parameters and have dual X and Y axes.

Under the **Axes** tab, you can specify the settings for the X and Y axis for the plot.



You must specify the starting and end dates for the **Time** (X) **Axis**. When you access the combo box in the **Minimum** or **Maximum** field, a mini windows calendar will appear as shown below.

This will allow you to quickly choose the date for the plot. Use the and arrows to move back or forward through the calendar. Alternatively, you can simply enter the time in the field by typing it in manually.

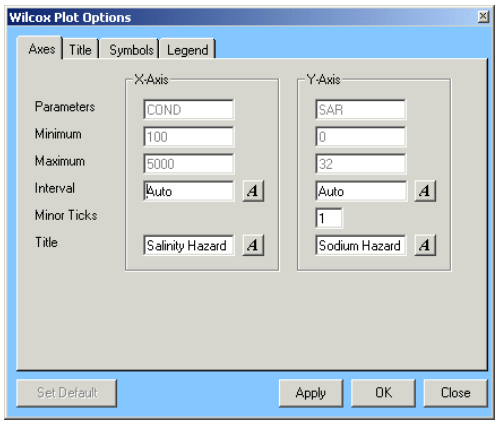
Below this, you can choose different options for the **Interval** and **Minor Ticks**. Time increments in days, weeks, months, or years are available. Finally, beside the **Format** field, you can choose the display format for the date.

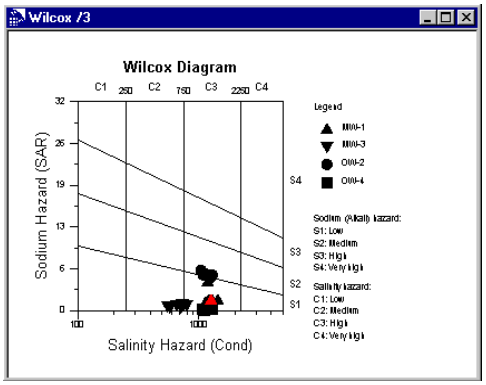
NOTE: The MMM indicates “full month name” e.g. May

Information on the remaining plot features can be found in the **Common Plot Features** section at the beginning of this chapter.

4.5.17 Wilcox Plot

A Wilcox plot can be used to quickly determine the viability of water for irrigation purposes. The Wilcox plot is also known as the U.S. Department of Agriculture diagram. An example of the **Wilcox** plot and the corresponding **Wilcox Plot Options** dialogue is shown in the figure below.





The Wilcox plot is a simple scatter plot of **Sodium Hazard** (**SAR**) on the **Y-axis** vs. **Salinity Hazard** (**Cond**) on the **X-axis**. The Conductivity (**COND**) is plotted by default in a log scale. These plot parameters are hardwired into AquaChem and cannot be changed. You must have values for the COND and SAR parameters in your database, in order to use this plot.

The Wilcox plot has the following sections:

Conductivity (us/cm)
C1: Low (0-249)
C2: Medium (250-749)
C3: High (750-2249)
C4: Very High (2250-5000)

The SAR values are divided into the following categories:
S1: Low
S2: Medium
S3: High
S4: Very High

The locations of the SAR lines are determined by the following equations:

S1: Line equation: y= -1.5816e-3x + 10.15816
S2: Line equation: y= -2.2959e-3x + 18.22959
S3: Line equation: y= -3.0102e-3x + 26.30102

5

Reports

When you select **Reports** from the main menu, you are presented with several types of reports to aid in the presentation of your data. These reports are generated in a separate Report window as unformatted text. These reports can be printed 'as is' using the **[Print]** button located on the lower-left corner of the report window, or the information can be easily saved using the **[Save]** button.

The following pre-defined Reports are included with AquaChem:

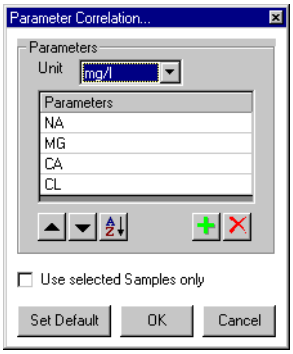
- Compare Samples
- Reliability Check
- Correlation Matrix
- Rock Source Deduction
- Mix Samples
- Statistics
- Water Quality Standards

In addition to these Reports, AquaChem v.4.0 allows you to design your own report templates, allowing you to produce reports on a wide variety of sample data and calculations. You can do so using the **Report Designer**; this component is explained further at the end of this chapter. AquaChem includes a **Sample Summary Report**, which was designed using the Report Designer.

5.1 Common Report Features

Although each pre-defined report has unique characteristics, there are also a few buttons and options that are common for all reports. These buttons may be found below the **Parameters** list in the **Report Options** dialogue, or in the **Report** window itself.

A generic Report options dialogue is shown below:



In most Report options, you will find the following buttons:

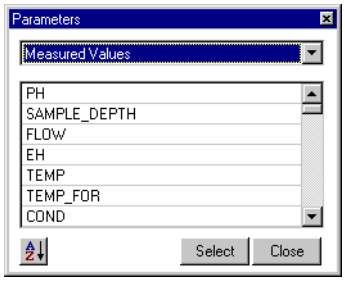
The up arrow button allows you to move the selected parameter up in the report options dialogue.

The down arrow button allows you to move the selected parameter down in the report options dialogue.

The sort button allows you to sort the parameter list alphabetically.

The delete button will remove the selected parameter from the parameters list.

The add button allows you to select a parameter from the list of available parameters and add new parameters to the Report. When you press the add button, the following dialogue will appear:

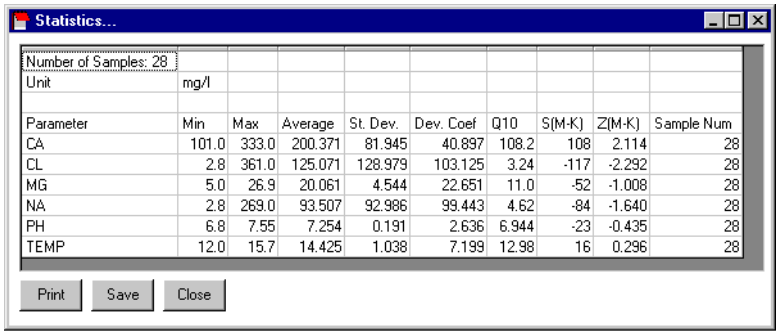


Simply choose the desired parameter and press the **[Select]** button, and this parameter will be included in the report. You can use the  button to sort the parameter list alphabetically, allowing you to quickly locate a parameter. In addition, some reports allow you to choose from several parameter categories, which are available in the combo box at the top of the **Parameters** dialogue. Once you are finished, press the **[Close]** button to close this dialogue.

When the **[Set Default]** button is pressed, the current parameter settings will be used as the default parameter settings for all new reports for the selected report type.

The **Select sample** button loads your list of active samples, and allows you to select a sample for the Report. ***Double-click*** on the desired sample to load this into the Report options.

A generic report window is shown below:



In most Report windows, you will find the following buttons:

The scroll buttons allow you to generate a Report for other samples in your active list. These buttons can be found on the bottom of the Report window. The function of these buttons (in order from left to right) is as follows:

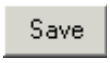
First sample - loads a Report for the first sample in your active list.

Previous sample - loads a Report for the previous sample in your active list.

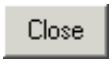
Next sample - loads a Report for the next sample in your active list.

Last sample - loads a Report for the last sample in your active list.

The **[Print]** button will print the current report to the selected Windows printer.



The **[Save]** button will save the current report. The pre-defined reports in AquaChem can be saved as .TXT and .CSV. The customized reports (designed using the Report Designer) can be saved as .HTM or .RTF format.



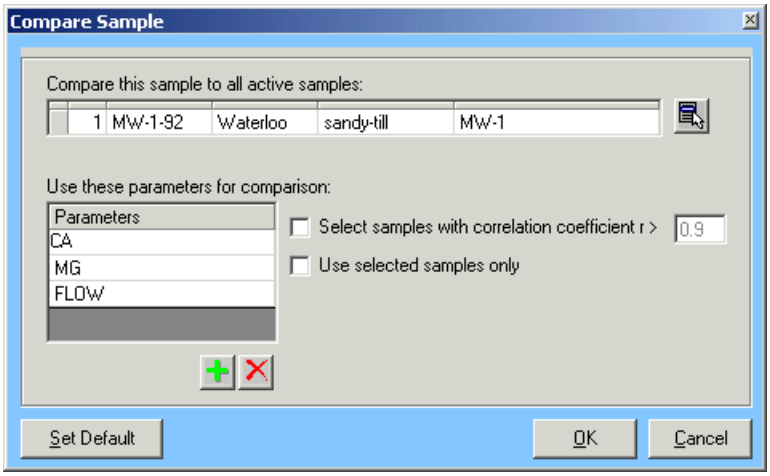
The **[Close]** button will close the Report window.

Where applicable, you can access the Report options dialogue by selecting **View** from the main menu and then **Options**. This allows you to change the report settings (such as which parameters or samples to use).

The following section provides more details on each of the various pre-defined Reports available in AquaChem.

5.2 Compare Samples

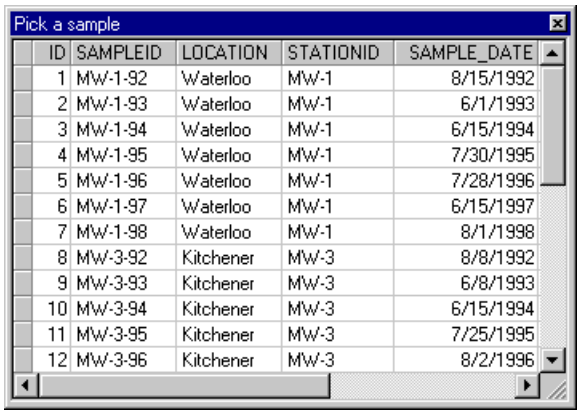
The Compare Samples report allows you to compare parameters for one sample to other samples in your database. This allows you to quickly determine the similarities or differences between your samples. When you select **Reports** from the main menu and then **Compare Samples**, the following dialogue will appear:



The top field in this dialogue "**Compare this sample to all active samples**" allows you to select a sample to be used in the report.

Press the **Select sample** button at the right side of this field and **Pick a Sample** dialogue will open up (as shown below). It allows you to select a sample for the Report.

.



ID	SAMPLEID	LOCATION	STATIONID	SAMPLE_DATE
1	MW-1-92	Waterloo	MW-1	8/15/1992
2	MW-1-93	Waterloo	MW-1	6/1/1993
3	MW-1-94	Waterloo	MW-1	6/15/1994
4	MW-1-95	Waterloo	MW-1	7/30/1995
5	MW-1-96	Waterloo	MW-1	7/28/1996
6	MW-1-97	Waterloo	MW-1	6/15/1997
7	MW-1-98	Waterloo	MW-1	8/1/1998
8	MW-3-92	Kitchener	MW-3	8/8/1992
9	MW-3-93	Kitchener	MW-3	6/8/1993
10	MW-3-94	Kitchener	MW-3	6/15/1994
11	MW-3-95	Kitchener	MW-3	7/25/1995
12	MW-3-96	Kitchener	MW-3	8/2/1996

Double-click on the desired sample to load this into the Report options.

The **Compare Sample** report requires you to specify **Parameters** which will be used in the comparison analysis. To add new parameters, press the button and select a parameter from the available list. You may also include parameter ratios, sums or differences (e.g. Na/Cl, Ca+Mg, Cl-SO4) in the Parameters field; simply type these values in manually in the parameter field. To remove parameters from the list, press the button. The default parameter settings for this report can be changed by modifying the parameters field and pressing the **[Set Default]** button in the lower left corner of this dialogue.

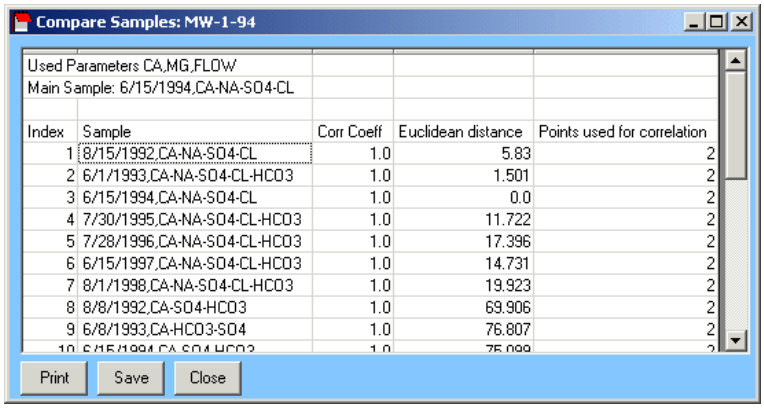
There are two options to select the samples from the active list:

- Select samples with correlation coefficient > #
- Use selected samples only

The **Select samples with correlation coefficient > #** option allows you to enter a correlation coefficient (r) value, and AquaChem will highlight (select) those samples in the active list once the comparison is completed.

When the **Use selected samples only** option is enabled, the Report will use only those samples that are selected (highlighted) in the active samples list, as part of the analysis.

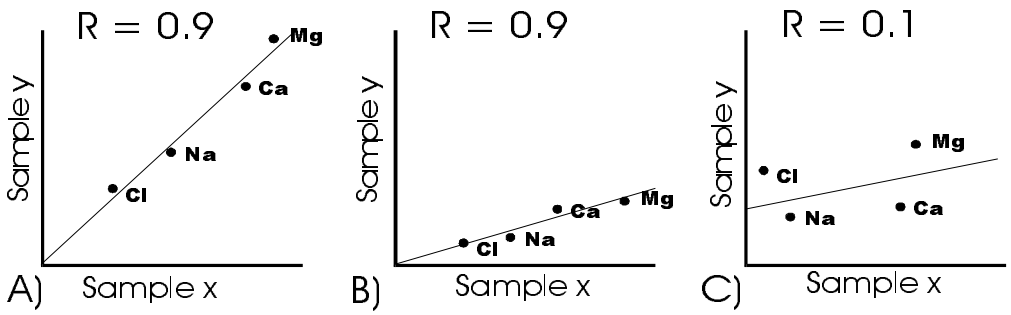
Once you have specified the required options, press **[OK]** and the report will be generated. An example is seen below:



The Compare Samples report uses a linear regression algorithm to generate the correlation coefficient and the Euclidean distance between a selected sample and all other active or selected samples. Samples having a chemical composition similar to the selected sample will have a correlation coefficient close to 1. The correlation coefficient is a function of ratios rather than absolute values. The difference in absolute concentrations is expressed by the Euclidean distance:

$$d_{ij} = \frac{\sum_{k=1} x_{ik} - x_{jk}}{n}$$

where x_{ik} denotes the *kth* variable measured on sample *i* and x_{jk} is the *kth* variable measured on sample *j*. For each sample, *n* variables are measured. The distance between sample *i* and sample *j* is d_{ij}.

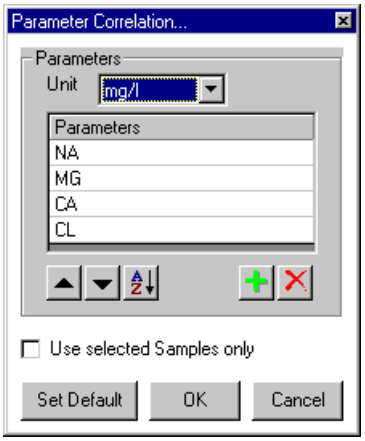


In the examples above, comparing **Sample x** to **Sample y**, the following conclusions can be made:

(A) high similarity
(B) high similarity but sample y is diluted with respect to sample x
(C) low similarity

5.3 Correlation Matrix

The Correlation Matrix Report shows a simple correlation matrix of the parameters for the samples in your database. This allows you to quickly determine the similarities or differences between your samples. When you select **Reports** from the main menu and then **Correlation Matrix**, the following dialogue will appear:

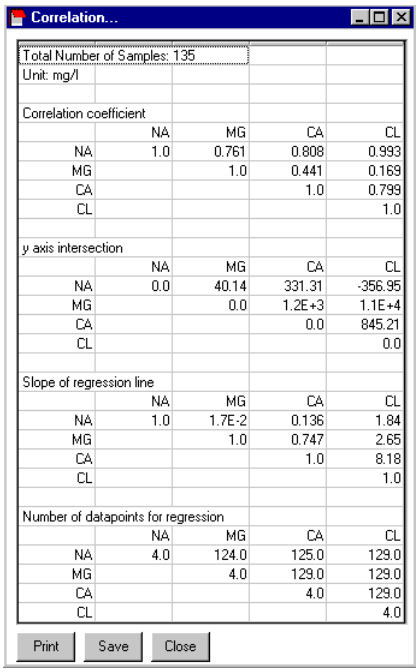


The Correlation Matrix Report requires you to specify parameters which will be used in the correlation analysis. To add new parameters, press the button and select a parameter from the available list. You can also include parameter ratios, sums or differences (e.g. Na/Cl, Ca+Mg, Cl-SO4) in the Parameters field; simply type these values in manually in the parameter field. To remove parameters from the list, press the button.

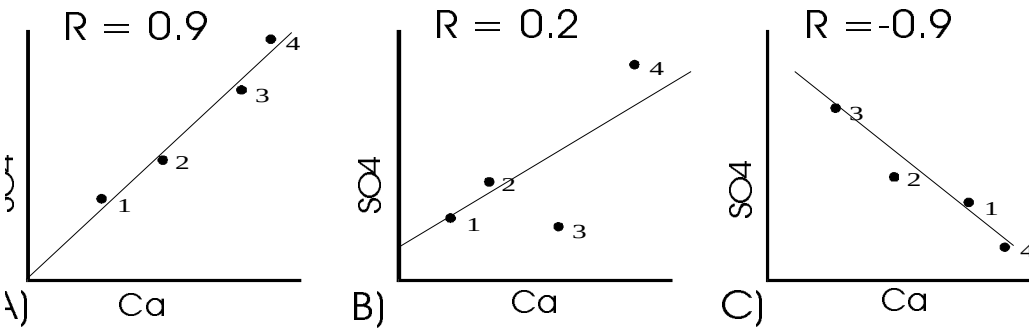
When the **Use Selected samples only** option is enabled, only the samples which are selected in the active list will be used. If this option is disabled, then all samples in the active list will be used.

The **Unit** field contains a combo box listing the available concentration units for the correlation of the chemical parameters. Units of **mol/l** are often more suitable for correlating than mg/L because it gives you an idea of which minerals have been dissolved.

Once you have specified the required options, press **[OK]** and the report will be generated as shown in the figure below:



The Correlation Matrix report generates a correlation matrix for a specified number of sample parameters that are common to all samples. A linear regression routine calculates the regression coefficient (r), and the slope and intercept of the regression line. The figure below shows the correlation of **Ca** against **SO4** for three different scenarios.



The correlation of Ca and SO4 in three samples above is as follows:

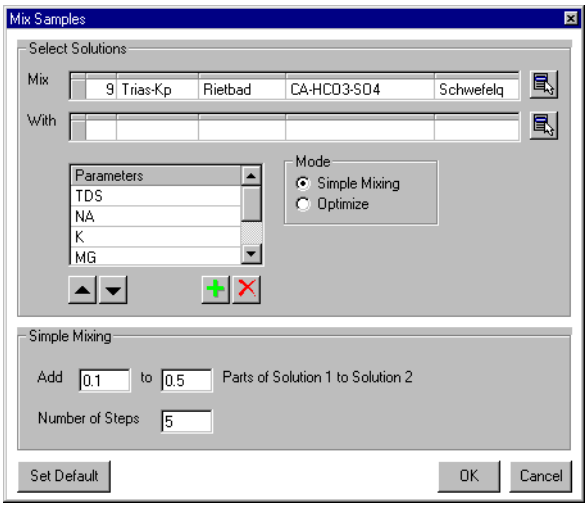
(A) high correlation
(B) low correlation
(C) high negative correlation

It is often useful to check the correlation results graphically in a scatter plot to easily identify outliers. The **Scatter** plot is available as one of the plot types, under the **Plots**

menu. In the Scatter plot options, access the **Edit Lines** option under the **Symbols** tab. In this dialogue, you can calculate the regression curve. For more details, see Scatter Plot in Chapter 4.

5.4 Mix Samples

The Mix Samples Report generates solution concentrations resulting from the step-wise mixing of specified proportions of two selected samples from your database. When you select **Reports** from the main menu and then **Mix Samples**, the following dialogue will appear:



In the **Select Solutions** frame, press the button beside **Mix** and **With** fields to select a sample from the available solutions (samples) that are in your database. Each field contains a complete list of all active samples in your AquaChem database.

The **Parameters** list allows you to select the parameters that will be included in the mixing calculations. Typically you should select parameters that you know are common to each sample. (If you use parameters which are not common to both samples, then the report may not be successfully generated). To add a parameter to the list, press the button and select a parameter from the list. To remove a parameter, select the parameter then press the button. The default parameter settings for this report can be changed by modifying the parameters and pressing the **[Set Default]** button in the lower-left corner of the dialogue.

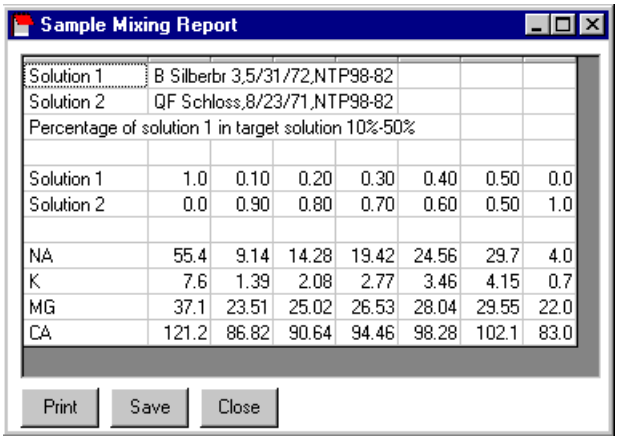
In the **Mode** frame there are two mixing options, the **Simple Mixing** mode and the **Optimize** mode. Each mode is described in detail below.

Simple Mixing Mode

When you select the **Simple Mixing** mode, AquaChem will mix the two selected samples in a step-wise process.

In the **Simple Mixing** frame, the **Add** field is the starting proportion (*m*) of Solution 1 in the mixture solution, while the **to** field is the final proportion (*n*) of Solution 1 in the mixture solution. The **Number of Steps** value is the number of uniform steps in which to get from (*m*) to (*n*) parts of Solution 1 in the mixture solution. Starting with (*m*) parts of Solution 1 and (1.0 - *m*) parts of Solution 2 in the mixture solution, AquaChem will begin uniformly decreasing the proportion of Solution 1 in the mixture solution while maintaining a total proportion value of 1.0. The final mixture solution has (*n*) parts of Solution 1 and (1.0 - *n*) parts of Solution 2.

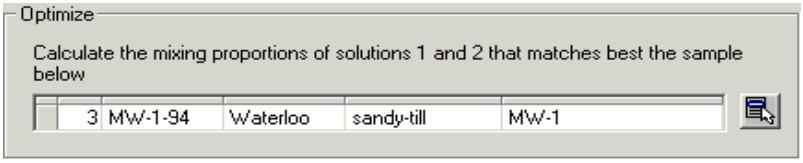
The figure below shows the **Sample Mixing Report**, and the results of mixing two solutions.



The concentrations of each parameter in the first column are the concentrations for Solution 1. The concentrations of each parameter in the second column are the concentrations for a mixture of 0.1 parts Solution 1 with 0.9 parts Solution 2. The concentrations of each parameter in the third column are the concentrations for a mixture of 0.2 parts Solution 1 with 0.8 parts Solution 2, and so forth for the remaining columns.

Optimize Mode

In addition to simple mixing of two samples, AquaChem also allows you to determine the optimal mixing ratio of the two selected samples that most closely matches a target sample from the database. When you select the **Optimize** mode, you will see the following options (in the lower half of the Report options dialogue):



This mixing mode requires you to select a sample that you would like to match. AquaChem will mix the two initial samples in 2% increments until the Euclidean distance between the calculated mixture and specified resulting sample is minimized.

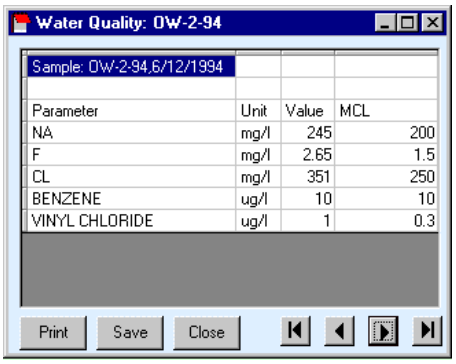
The **Optimize** mode can be used in a situation where you have three samples (ex. groundwater, seawater and freshwater) and you suspect that the groundwater is a mixture of the freshwater and the seawater. The **Optimize** mode can be used to estimate the percentage of freshwater and the percentage of seawater required to obtain the groundwater composition of selected parameters.

To generate a report with Optimize mode, select a sample from your database, and click **[OK]**.

5.5 Water Quality Standards

The **Water Quality Standards** report provides a list of all parameters which exceed one or all of the established Guideline/Tolerance levels for the selected sample. If your sample contains no exceedences, then this Report will be blank.

When you select this report, a **Water Quality** window similar to the one below will appear:



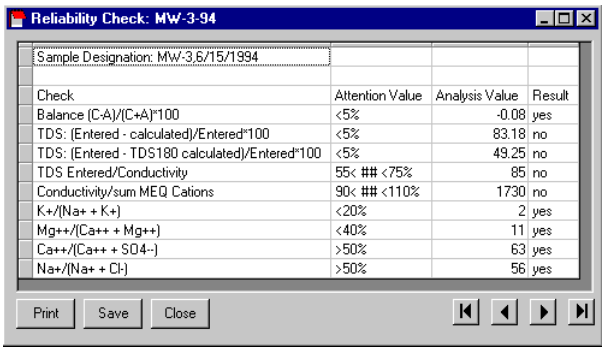
Each line of the report contains the **Parameter**, corresponding **Unit**, actual measured **Value** and guideline values (**MCL**, **GLL2**). Depending on the Guideline used, you may see one, two, or three guideline levels. The example above shows two levels, a

recommended tolerance interval and a maximum tolerance interval. The default settings for the report are in accordance with the guidelines specified in the **Preferences** dialogue available under the **File** menu.

The scroll arrows in the lower right corner of the Report window can be used to produce a report for other samples in your database.

5.6 Reliability Check

This Reliability Check Report helps you to confirm the validity of the measured sample data. When you select this report, the following **Reliability check** window will appear:



This report provides a number of checks which can provide insight on the reliability of the water sample analysis. If the analysis value passes the test, then a Yes will be displayed in the **Result** column; if not, then a No will be displayed. Each analysis is explained in the Table below:

Available Tests in the Reliability Check Report

Test	Attention Value	Comments
Balance (C-A)/(C+A)*100	<5%	The solution must be electrically neutral or within ±5 : sum of cations = sum of anions.
TDS: [(Entered-calculated)/Entered]*100	<5%	Calculated TDS = sum ions (mg/L) + SiO2 must be similar to measured dry residue.
TDS: [(Entered -TDS180^{o} calculated)/ Entered]*100	<5%	Calculated TDS = sum ions (mg/L) + SiO2 - 0.5082 * bicarbonate. Must be similar to measured dry residue at 180°.
TDS Entered/Conductivity	0.55 < x < 0.75	There is a linear relation between TDS and conductivity within a range of 0.55 to 0.75.

Available Tests in the Reliability Check Report

Conductivity/Sum MEQ Cations	90 < x < 110	There is a linear relation between Conductivity and Sum of Cations within a range of 90 - 110.
$K^+/[Na^+ + K^+]$ meq/l	<20%	Na >>K
$Mg^{++}/[Ca^{++} + Mg^{++}]$ meq/l	<40%	Ca > Mg, unless provided by the dissolution of dolomite.
$Ca^{++}/[Ca^{++}+SO4^{--}]$	<50%	Most SO4 concentration can be attributed to the dissolution of gypsum. Therefore the Ca/SO4 ratio must be 1:1 or lower, if some Ca is also provided by the dissolution of carbonate.
$Na^+/(Na^+ + Cl^-)$	>50%	Chloride is mainly provided by the dissolution of Halite (NaCl). Therefore the ratio Na/Cl is 1 or higher, if some Sodium is added to the solution by the solution of silicates or by ion exchange.

NOTE: Some attention values are displayed as "acceptable ranges". This means that the Analysis value must be within this range. The analysis (calculated) values can be positive or negative. If the analysis values are outside this range (either positively or negatively) then the value will not "pass" this check, and the report will display a "NO", indicating that the sample did not pass this analysis check.

If the calculated values are not within the attention values (i.e. the Result is No), then this does not necessarily signify an error; it does mean however that there should be an explanation for the value. For example, if Na/Cl< 1 then the explanation could be that some Na has been removed from the solution by Na > Ca exchange: this should be confirmed by a suitable aquifer geology (exchange friendly minerals such as Ca-rich clay). Ca/SO4 < 1 can be explained by the dissolution of ferrous minerals such as pyrite. This effect is often observed in mine tailings. However, normal groundwater samples should fulfill all the criteria mentioned above.

The scroll arrows in the lower right corner of the **Reliability check** window can be used to produce a report for other samples in your database.

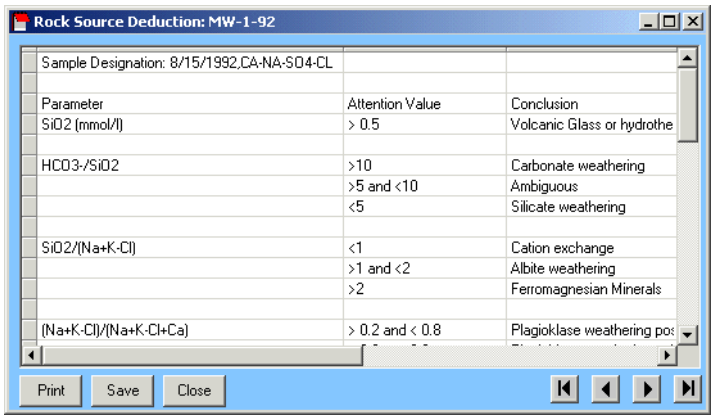
For more details please see the reference below:

Hounslow, A.W. 1995. *Water Quality Data – Analysis and Interpretation*. CRC Press LLC. p.75.

5.7 Rock Source Deduction

The Rock Source Deduction report allows you to gain insight into the possible origin of the water sample. The results are a general overview based on ion ratios found in a sample. If results do not meet expectations, the result should be confirmed with more detailed study based on multiple samples, aquifer mineralogy analysis, modeling and with the use of plots.

When you select this report, the following **Rock Source Deduction** window will appear:



The following table provides a summary of the criterion for the Rock Source Deduction Report.

Rock Source Deduction Analysis

Parameter	Attention Value	Conclusion	Comments
SiO2 (mmol)	>0.5	Volcanic glass or hydrothermal water possible	The solubility of quartz at 20° is X mg/L.
HCO3-/SiO2	>10 >5 and <10 <5	Carbonate weathering Ambiguous Silicate weathering	Low carbonate SiO2 ratios indicate, that these ions are released from silicate minerals, especially if TDS is low.
SiO2/(Na+K-Cl)	<1 >1 and <2 >2	Cation exchange Albite weathering Ferromagnesian minerals	
(Na+K-Cl)/ (Na+K-Cl+Ca)	0.2 - 0.8 <0.2 or >0.8	Plagioklas weathering possible Plagioklas weathering unlikely	

Rock Source Deduction Analysis

Na/(Na+Cl)	>0.5 =0.5 <0.5 TDS >500 <0.5 TDS <500 and >50 <0.5 TDS <50	Sodium Source other than halite - albite, ion exchange Halite Solution Reverse Softening, seawater Analysis Error Rainwater	
Mg/(Ca+Mg)	=0.5 and (HCO3/Si)>10 <0.5 >0.5 <0.5 and (HCO3/Si)<5 >0.5	Dolomite Weathering Limestone-Dolomite Weathering Dolomite Dissolution, calcite precipitation, or seawater Ferromagnesian Minerals Granitic weathering	
Ca/(Ca+SO4)	=0.5 <0.5 and pH<5.5 <0.5 and pH neutral >0.5	Gypsum dissolution Pyrite oxidation Calcium removal - ion exchange or calcite precipitation Calcium source other than gypsum - carbonate or silicates	
TDS	>500 <500	Carbonate weathering or brine or seawater Silicate weathering	
Cl/Sum Anions	>0.8 and TDS>500 >0.8 and TDS<100 <0.8	Seawater or brine or evaporites Rainwater Rock weathering	
HCO3/ Sum Anions	>0.8 >0.8 and SO4 >20meq/L <0.8 and sulfate low	Silicate or carbonate weathering Gypsum dissolution Seawater or brine	
Calcite Saturation Index	>0 =0 <0	Oversaturated with respect to Calcite Saturated with respect to Calcite Undersaturated with respect to Calcite	

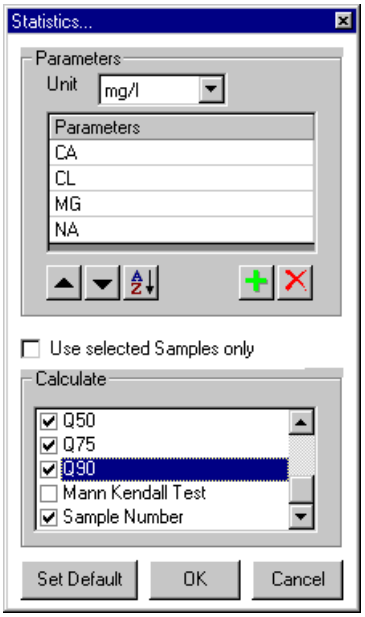
The report will complete the **Parameter** analysis, check the **Attention Values**, and produce a result value and **Conclusion** on the rock source.

The scroll arrows in the lower right corner of the **Rock Source Deduction** Report window can be used to produce a report for other samples in your database.

For more details please see the reference below:
Hounslow, A.W. 1995. *Water Quality Data – Analysis and Interpretation*. CRC Press LLC. p.85.

5.8 Statistics

The Statistics Report calculates basic statistics for all active or selected samples in your database. When you select **Reports** from the main menu and then **Statistics**, the following **Statistics** options dialogue will appear:



In this dialogue, the **Parameters** field allows you to select the parameters that will be included in the statistical analysis. To add a parameter to the list, press the button and select a parameter from the list. To remove a parameter, select the parameter then press the button. The default parameter settings for this report can be changed by modifying the parameters field and pressing the **[Set Default]** button in the lower left corner of the dialogue.

You can also include Parameter ratios, sums or differences (e.g. Na/Cl, Ca+Mg, Cl-SO4) in the **Parameters** field. Simply type these parameter combinations into the field manually with your keyboard.

The **Unit** field contains a combo box listing the chemical concentration units to be used in the statistical analysis. Chemical concentrations can be expressed in mg/L, mmol/l, meq/l, ppm or mol/L.

Statistics may be calculated for all active samples in the sample list, or only for those samples which are selected (highlighted) in the active list. To enable this option, place a check mark in the box beside **Use Selected Samples only**.

To study the influence of specific samples in your database, you can create multiple statistical reports using different selections of samples.

Under the **Calculate** frame (at the bottom of this dialogue), there is a list of the various statistical analysis available. To show the desired statistics on the report, place a check mark beside each analysis.

The following is a description of each Statistical Analysis available for this report:

Min (minimum): lowest recorded value for that parameter
Max (maximum): highest recorded value for that parameter
Average: average value for that parameter

St. Dev (Standard Deviation): calculated using the formula below

$$\sigma = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n}}$$

Dev. Coef. (Deviation Coefficient): Coefficient of Variance calculated using the formula below.

$$\frac{\sigma}{\bar{X}} \cdot 100$$

Q10: 10% of the samples lie below this value, for that parameter
Q25: 25% of the samples lie below this value, for that parameter
Q50: 50% of the samples lie below this value, for that parameter
Q75: 75% of the samples lie below this value, for that parameter
Q90: 90% of the samples lie below this value, for that parameter

Sample Number: number of samples that have a measured value for the selected parameter.

Mann-Kendall Test: The Mann-Kendall test is a trend estimator that can be used to prove if contaminant concentrations are significantly diminishing or rising over time. For this test, there are no distributional assumptions, and missing data (non-detects) or irregularly spaced measurement periods are allowed. Non-detects are assigned a value smaller than the smallest measured value.

The version of the **Mann-Kendall Test** used in AquaChem is recommended for 40 or less measurements and can be applied for virtually any groundwater parameter. The Mann Kendall test provides two values; S value and Z value.

The test procedure is as follows:

First, the data is ordered by sampling date $x_1, x_2, ...,x_n$ where x_i is the measured value on occasion i.
Second, record the signs of each of the N' possible differences $x_i' - x_i$ where $i' > i$. For example, let

$\text{sgn}(x_i' - x_i) = 1$ if $x_i' - x_i > 0$
$= 0$ if $x_i' - x_i = 0$

$= -1$ if $x_i' - x_i < 0$

The Mann-Kendall statistic (*S*) is then computed as:

$$S = \sum_{i=1}^{n-1} \sum_{i'=k+1} \operatorname{sgn}(x_{i'} - x_i)$$

which is the number of positive differences minus the number of negative differences.

If S = 0, then there is no increasing or decreasing trend in the data
If S < 0, then there is a decreasing trend, indicating concentration is decreasing over the time interval.
If S > 0, then there is an increasing trend, indicating concentration is increasing over the time interval.

A two-sided test (for either increasing or decreasing trend) can also be obtained, using probability values. For n > 10, then the normal approximation (*Z*) is calculated as follows:

If S > 0, then

$$Z = \frac{S-1}{[var(S)]^{0.5}}$$

If S = 0, then Z = 0

If S < 0, then

$$Z = \frac{S+1}{[var(S)]^{0.5}}$$

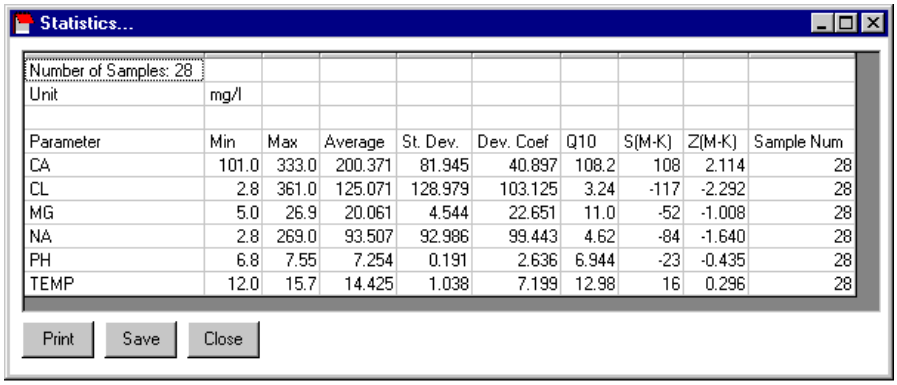
The quantity *Z* can be compared to standard normal cumulative distribution probabilities to test the null hypothesis of no trend.

Please note that ties (duplicate values), are not corrected when calculating the Z value.

In the Statistics Report window, the *S* value is displayed as S(M-K), and the *Z* value is displayed as Z(M-K).

For more details on the Mann-Kendall test please see the reference below:
Gibbons, R.D., 1995: *Statistical Methods for Groundwater Monitoring*. p.178.

Once you have specified the required report options, press **[OK]** and the report will be generated, as shown in the figure below:



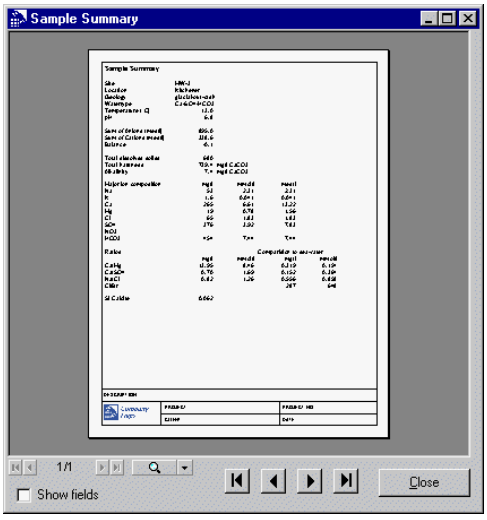
This report can now be saved or printed using the menu commands or the short cut buttons at the bottom of the report window.

5.9 Sample Summary

The Sample Summary report is formatted differently from the other reports described up to this point. This report was designed using the **Report Designer**; as such, you have the option to modify the appearance of this report, including the layout, available fields, and printing template. For more details on how to modify this report template, please see the **Report Designer** section at the end of this chapter.

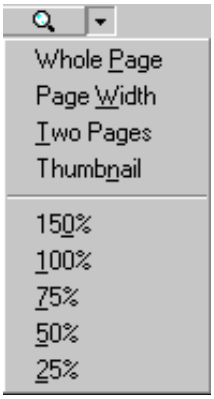
The Sample Summary Report provides a general overview of a sample including major ions, hydrochemical facies (e.g. Na-Cl), calculated hardness, ion balance, ion ratios, etc. The parameter values are read directly from the Sample Details window for each sample; this report shows both measured and calculated values.

When you select the **Reports** from the main menu and then **Sample Summary**, the following **Sample Summary** report window will appear.



The report window for user-defined reports (as shown in the figure above) has a few more options available at the bottom of the report window:

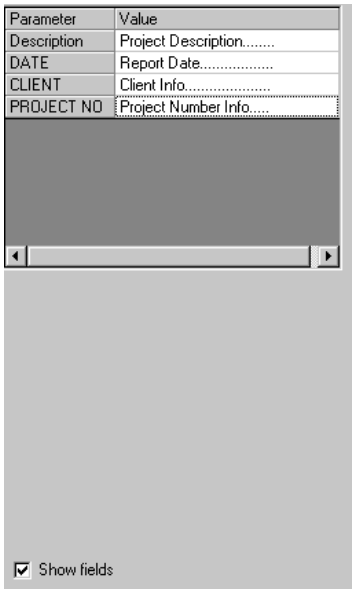
The **Scroll arrows** are only available when you have a report that contains multiple pages. The page count shows the current page number, out of the total number of pages available. The **Zoom** (magnifying) button allows you to change the zoom size of the window.



When you press the down arrow beside the magnifying glass, you will see several window size options. Simply choose the desired zoom size and the preview window should be automatically refreshed.

The **Show fields** option is only available if the Report is linked to a printing template (done using the Report Designer). To enable this option, place a check mark in this box. You will then see the following dialogue appear in the middle of your display, to the left of the preview window:

In these fields, you can enter the appropriate descriptive information for the report. As the information is entered, the report preview window should be automatically updated.



Once you are finished, you may print or save the report. The user-defined reports allow you to print a report for multiple samples. To do this, simply select multiple samples from your sample list, and generate the sample summary report. The printout will contain a report for each selected sample. In addition, you can save this report, and the saved file will contain a report for each of the selected samples. This report can be saved as .HTM or .RTF format.

NOTE: When you save user-defined reports, the report template information will not be saved; only the report contents are saved to a file.

5.10 Report Designer

As mentioned earlier in this chapter, AquaChem allows you to create two types of reports:

- The pre-defined (hardwired) reports, and
- The user-defined reports

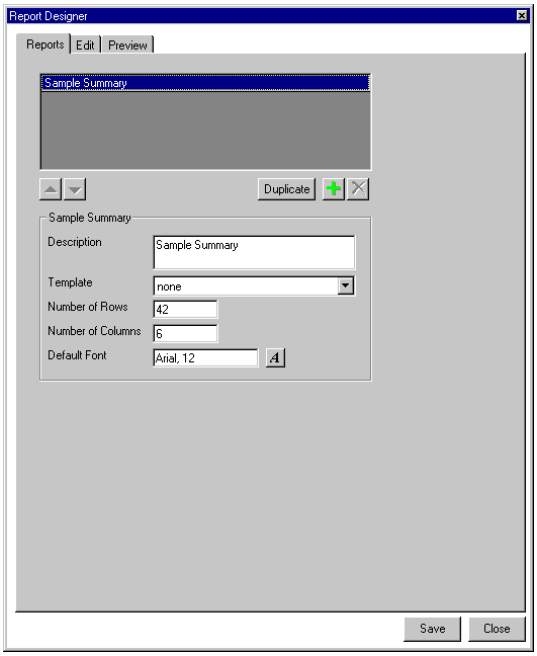
The hardwired reports cannot be modified, nor can their layout be changed. These reports include: Compare Samples, Correlation Matrix, Mix Samples, Water Quality Standards, Reliability Check, Rock Source Deduction, and Statistics.

The user-defined reports (ex. Sample Summary) can be modified using the **Report Designer**.

Using the **Report Designer** you may design and customize up to 10 new reports for your own project needs. The report may include any combination of database parameters and function (calculation) results. Once a new report has been created, it can be selected from the **Reports** menu, below the **Sample Summary** report.

General Features

When you select **Reports** from the main menu and then **Report Designer**, the following dialogue will appear. The Report Designer dialogue is separated into three tabs: **Reports**, **Edit**, and **Preview**.



Reports

Provides a list of the reports available in the current database template, and general information on each report (Description, Selected Printing template, report size, and selected font).

Edit

Provides options for designing the report layout.

Preview

This tab provides you with a preview of the selected report.

You will also find the following buttons in the **Report Designer** dialogue.

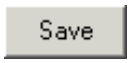
The up-arrow button allows you to change the order of the selected reports upwards as they appear in the **Reports** menu (in the main menu).

The down-arrow button allows you to change the order of the selected reports downwards as they appear in the **Reports** menu (in the main menu).

The add button creates a new report.

The delete button deletes the selected report.

The **[Duplicate]** button creates a duplicate copy of the selected report. This allows you to quickly modify an existing report, without having to create a new one from scratch.



The **[Save]** button at the bottom of the dialogue saves the current report information.

The **[Close]** button closes the Report Designer dialogue.

In order to quickly learn the functionality of the Report Designer, an example has been provided below.

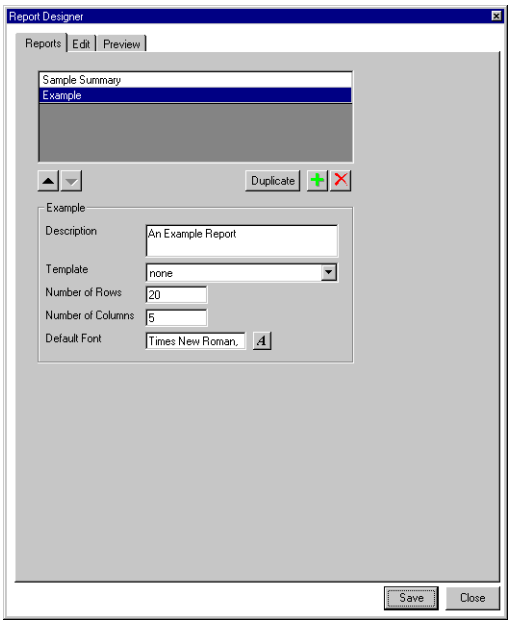
Designing a New Report - Example

Before customizing a report you should create a spreadsheet-style layout of this report using a program such as Excel. Decide what fields you want to use, their placement, and how wide the cells need to be. This will speed-up the process when using the Report Designer in AquaChem. Below is the layout that will be used for this simple example report.

	A	B	C	D	E
1	General Report				
2					
3	Sample ID				
4	Sampling Date				
5	Location				
6					
7	Major Ions				
8		mg/L		mg/L	
9	Ca		CL		
10	Mg		SO4		
11	Na		HCO3		
12					
13	Sum Anions		Sum Cations		
14	Ion Balance				
15					
16	Ratio	mg/L			
17					
18	NA/CL				

To create a new report, follow the steps as described below.

If you have not already done so, load the **Report Designer** from the **Reports** menu. Ensure you are viewing the Reports tab (the first tab).



☞  button to create a new report. A new line will be added below the **Sample Summary** Report at the top of the dialogue, with the name: **#New Report**.

☞☞ **#NewReport** and enter a name for this new report.

type: **Example**

☞ **<Enter>** (on your keyboard)

In the lower half of this dialogue:

type: **An Example Report** (in the **Description** field)

☞ '**none**' for the Template

type: **20** (the Number of Rows for this report)

type: **5** (the Number of Columns for this report)

☞  button to change the Default Font for this report

☞ Times New Roman / Regular / 10 font size

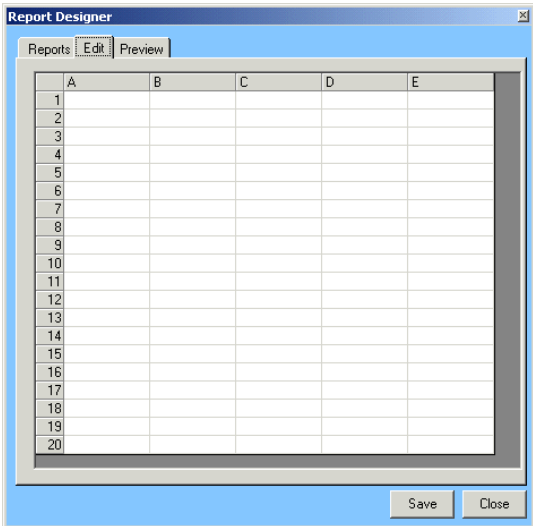
☞ **[OK]**

☞ **[Save]** (in the lower right corner of the dialogue) to save this report.

You can now proceed to add fields to this report.

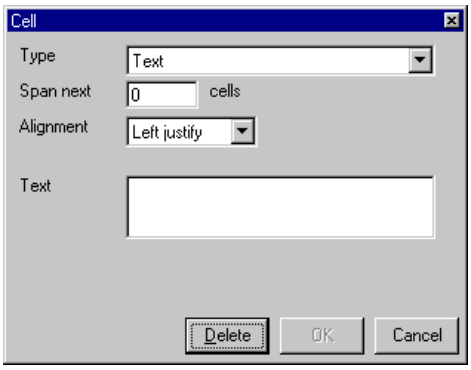
☞ **Edit** tab (from the top of the dialogue).

This will present you with a blank grid (spreadsheet), containing 20 rows and 5 columns as shown below.



You will see that the rows are numbered and the columns are lettered (similar to MSExcel) to allow you to quickly locate cell locations in the grid. At this point you may begin to add values to the cells. You may fill cells with text, database parameters, or with a function (calculation).

☞☞ ***Double-click*** on the cell in the upper-left corner (Cell **A1**) and the **Cell** dialogue (as shown below) will appear:



This dialogue allows you to control the contents of the selected cell. Cell contents must be assigned one cell at a time. Below are the options available for each cell:

Type

Click on the ▼ button and you may choose from the following cell types:

Text: Enter the desired text for the cell
Sample Description: choose from a list of Sample Description parameters
Station Description: choose from a list of Station Description parameters
Measured/Modeled Value: choose from a list of Measured or Modeled parameter values.
Ratio: choose two parameters to show as a ratio
Guideline Level1: displays the current guideline level 1 for the specified parameter
Guideline Level2: displays the current guideline level 2 for the specified parameter
Function Value: choose from a list of available calculations
Range Name: select from a list of available Ranges
Thermometers: select from a list of Geothermometers

Span next

This option is useful for headings and titles, where the text may not fit into one cell. If the cell to the right of the selected cell is empty, you may span several cells into one. Simply enter a cell number in this field (ex. Span 2 cells).

Alignment

Choose from Left, Center, or Right-Justified.

Parameter

Value for the cell.

Unit

Choose from common measurement units.

Format

Choose the display format for the cell.

> **NOTE:** The cell dialogue will have various options depending on the cell **Type** that is selected.

You will now enter a Report Title for cell A1:

☞ **Text** (from the list beside the **Type** field)

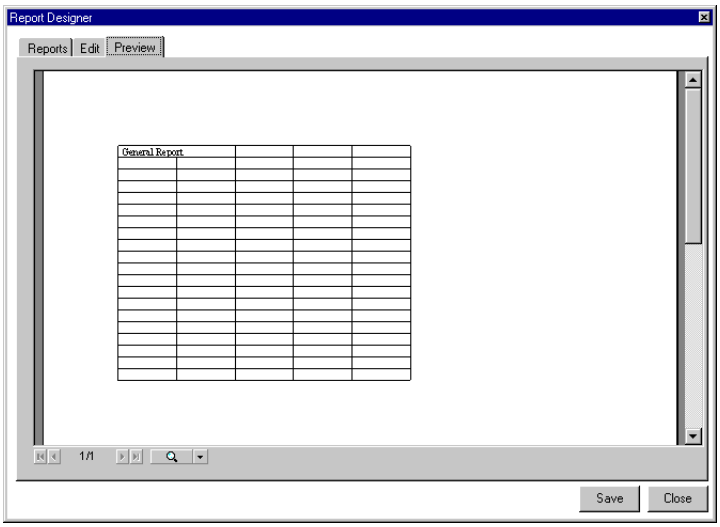
type: **1** beside the **Span next cells** field

☞ **Left justify**, for the cell alignment

type: **General Report** (beside the **Text** field)

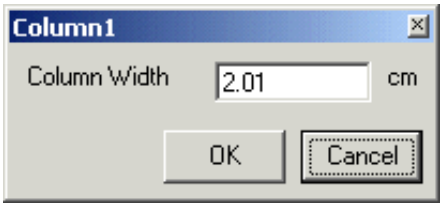
☞ **[OK]**

You should now see an entry under the **Edit** tab for Cell **A1**. You may switch to the **Preview** tab to see a preview of how the report will appear.



The colors of the cells in the **Edit** dialogue are representative of the cell types. The following summary provides a list of what each cell color indicates of the cell type:

Black: Text cells
Green: Sample and Station Description parameters
Blue: Measured and Modeled parameters, and Parameter Ratios
Grey: Function (Calculated) values, Thermometers, and Ranges
Red: Guideline Levels



If you want to change the column widths, simply drag the column to the desired width in the spreadsheet. Alternatively, you can select the column then right-click the highlighted column to **Set Column Width**. Enter the precise value of the column width in the pop-up dialogue and press **[OK]**. Then load the **Preview** window to see the refreshed report.

The font for the report may be customized in two places:

In the **Reports** tab, the **Default Font** for the entire report is defined; all items on the report will use this font, size and style.

A default font may also be assigned on a per row basis. To do so, select an entire row and right-mouse click on it. Select the desired **Font** from the options that appears, and

click **[OK].** This font will be applied to an entire row. This is practical for assigning fonts to column headings in the report.

You will now proceed to define the remaining cells in the report, as per the pre-designed layout:

☞ **Edit** tab, from the top of the **Report Designer** dialogue.

☞☞ Cell **A3**

☞ Select **Text** from **Type** field

type: **Sample ID**

☞ **[OK]**

☞☞ Cell **A4**

☞ Select **Text** from **Type** field

type: **Sampling Date**

☞ **[OK]**

☞☞ Cell **A5**

☞ Select **Text** from **Type** field

type: **Location**

☞ **[OK]**

Using the same procedure, fill in the remaining text fields as per the layout above, in the appropriate cell locations:

Cell	Text Entry
A7	**Major Ions**
A9	**Ca**
A10	**Mg**
A11	**Na**
A13	**Sum Anions**
A14	**Ion Balance**
A16	**Ratio**

A18	**NA/CL**
B8	**mg/L**
B16	**mg/L**
C9	**Cl**
C10	**SO4**
C11	**HCO3**
C13	**Sum Cations**
D8	**mg/L**

Once you are finished you should save the changes that have been made so far.

- ☞ **[Save]** in the lower-right corner of the **Report Designer** dialogue, to save the report design changes up to this point.

You can now add in the parameter value cells and function values.

- ☞☞ Cell **B3**
- ☞ **Sample Description** from the combo box beside cell **Type**
- ☞ **SAMPLEID** from the combo box beside **Sample Parameter** field
- ☞ **[OK]**
- ☞☞ Cell **B4**
- ☞ **Sample Description** from the combo box beside cell **Type**
- ☞ Select **SAMPLE_DATE** from the combo box beside **Sample Parameter** field
- ☞ **[OK]**
- ☞☞ Cell **B5**
- ☞ **Station Description** from the combo box beside cell **Type**
- ☞ Select **LOCATION** from the combo box beside **Station Parameter**
- ☞ **[OK]**

Notice the color of the cells under the **Edit** tab in the **Report Designer** dialogue for these new cells; green cells indicate that these cells contain Station/Sample Description parameters.

☞☞ Cell **B9**

☞ **Measured /Modeled Value** from the combo box beside cell **Type**

☞ **Ca** from the combo box beside **Parameter**

☞ **mg/l** from the **Unit** field

☞ **[OK]**

☞☞ Cell **B10**

☞ **Measured Modeled Value** from the combo box beside cell **Type**

☞ **Mg** from the combo box beside **Parameter**

☞ **mg/l** from the **Unit** field

☞ **[OK]**

☞☞ Cell **B11**

☞ **Measured Modeled Value** from the combo box beside cell **Type**

☞ **Na** from the combo box beside **Parameter**

☞ **mg/l** from the **Unit** field

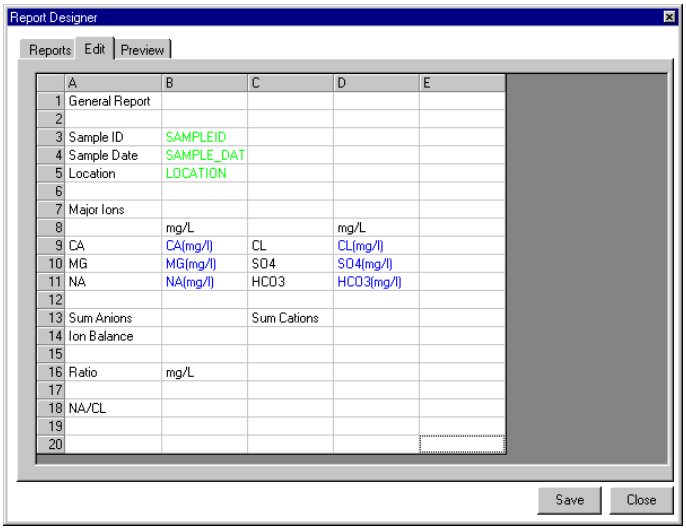
☞ **[OK]**

Notice the color of the cells in the **Edit** dialogue; blue cells indicate that these cells contain Measured values.

Repeat this step for the remaining ions by choosing the appropriate parameter and placing this in the cell immediately beside the text cell for that parameter.

Cell	Measured Value
D9	**Cl**
D10	**SO4**
D11	**HCO3**

Once you have finished this step, your display should be similar to the one shown below:



☞ **[Save]** in the lower-right corner of the **Report Designer** dialogue to save the report design changes up to this point.

You will now add function values for the Sum Anions, Sum Cations, and Ion Balance

☞☞ Cell **B13**

☞ **Function Value** from the combo box beside cell **Type**

☞ **Left Justify** from the **Alignment** field

☞ Select **Sum of Anions** from the combo box beside **Function**

☞ **[OK]**

☞☞ Cell **D13**

☞ **Function Value** from the combo box beside cell **Type**

☞ Select **Sum of Cations** from the combo box beside **Function**

☞ **[OK]**

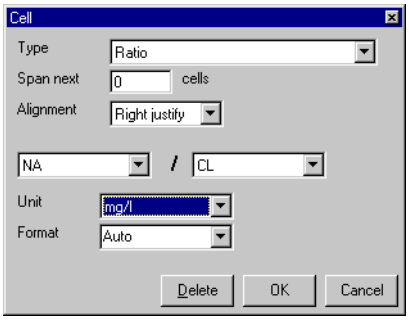
☞☞ Cell **B14**

☞ **Function Value** from the combo box beside cell **Type**

☞ **E. N.** (Electroneutrality) from the combo box beside **Function**

☞ **[OK]**

Notice the color of the cells in the **Edit** dialogue; grey cells indicate that these cells contain Function (Calculated) values. Finally, you will add a Ratio to Cell B18 showing a parameter ratio of NA / CL.



☞☞ Cell **B18**

☞ Select **Ratio**, from the combo box beside cell **Type**

☞ **Na** for the first parameter

☞ **Cl** for the second (right) parameter

☞ **mg/l** for the units

☞ **[OK]**

Notice the color of the cells in the **Edit** dialogue; blue cells indicate that this cell contains a Parameter Ratio.

☞ **[Save]** in the lower-right corner of the report designer dialogue to save all changes to this report.

Once you have designed the report, click on the **Preview** tab to see a page preview.

This concludes the steps required to design a report. Feel free to add new cell values, functions, parameters, etc. in order to see the full capabilities of the **Report Designer**.

Once you are finished in the **Report Designer**, press **[Close]** to return to the main window of AquaChem. The newly created "**Example Report**" will now be available under **Reports** in the AquaChem main menu.

6

Tools

The **Tools** menu provides access to the AquaChem data analysis tools, including Converters, Calculators, LookUp Tables, and access to the PHREEQC modeling interface.

The following **Calculators and Converters** are available:

- AquaChem Function
- Decay Calculator
- Find Missing Major Ion
- Formula Weight Calculator
- Volume Concentration Converter
- Special Conversions
- Species Converter
- Unit Calculator

The following **LookUp Tables** are available:

- Degradation Rates
- PHREEQC Phases
- Periodic Table
- Adsorption Isotherms

Finally, under the **Modeling** options you may:

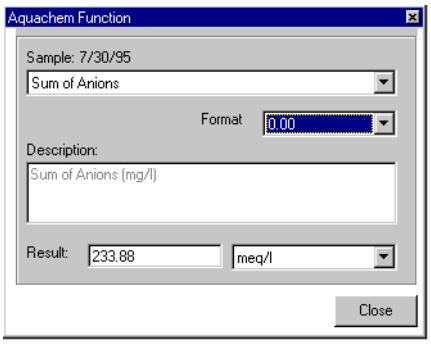
- Calculate Saturation Indices and Activities
- Calculate pH
- Calculate Eh
- Run a PHREEQC (Basic) Simulation
- Run a PHREEQC (Advanced) Simulation

6.1 Calculators and Converters

6.1.1 AquaChem Function

This tool allows you to quickly calculate any of the AquaChem Functions. Calculations can be performed without having to add/remove individual functions to the options of the Sample Details window.

To use this tool, first select a sample from your Active Samples list. Then select **Calculators > AquaChem Function** from the **Tools** menu, and dialogue will appear as shown to the right side.



In this dialogue, you can see a **Description** of the function and the function units. By clicking on the down-arrow key, choose a function and then **Format**, you will see the resulting value displayed in the **Result** field.

The calculations can be customized in the **Calculations** section of the **Database** options dialogue under the **File** menu. In here, you may select which calculations should appear in the AquaChem functions (calculations) lists.

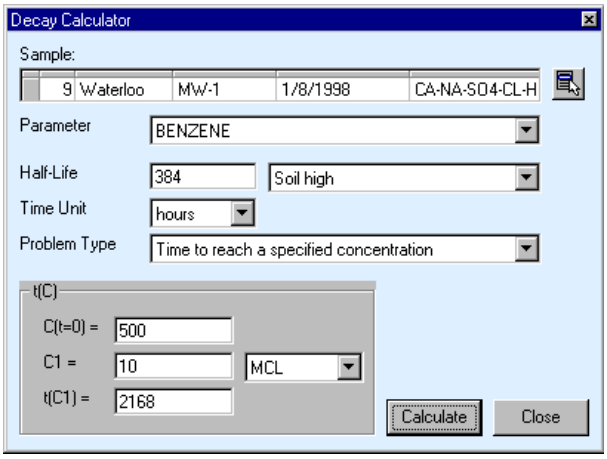
6.1.2 Decay Calculator

The Decay Calculator allows you to calculate the concentration of a contaminant following a specified time of decay, or the time to reach a specified concentration. Degradation rates of contaminants are usually given as "half-lifes", which is the time required for the substance to be reduced to half of the initial mass. This tool can be applied only to organic chemical parameters in your database. The formula for the rate of decay is as follows:

$C0/C1 = e^{-kt}$

Where,
t = time
C0 = initial concentration
C1 = concentration after time t

When you access this tool, the following **Decay Calculator** dialogue will appear. The components of this dialogue are described below.



Sample

At the top of this dialogue under the **Sample** field, click on button and then double-click in **Pick a sample** list to select a sample for which you would like to run a degradation analysis. Selecting a sample from the sample list copies the concentration value for the current parameter to the initial concentration field **C(t=0)**.

Parameter

In the **Parameter** field, click on the button and select the organic parameter you would like to analyze (please ensure that your sample contains a value for this organic parameter). Note that the parameter list contains all database parameters, which have a corresponding record in the **Degradation Rates** table (available under **Tools > LookUp Tables**).

Half-Life

After selecting a parameter, the **Half-Life** field will be automatically filled in with the appropriate value. The combo box to the right of the Half-Life field provides options for the Half-Life environments (**Soil**, **Air**, **Groundwater**, and **Surface water**) for which degradation rates are specified in the database. If all rates are known for these environments the list will contain a **high**, **low**, and **average** half-life values for each environment.

AquaChem includes values for 335 organic chemicals. These are taken from the following Reference:

Howard, P.H. et al., 1991: *Handbook of Environmental Degradation Rates*, Lewis Publishers, 775 p.

You may also use this tool as a simple degradation calculator, without selecting samples or parameters. Simply enter a **Half-life** value manually, choose your **Problem Type**, enter an initial concentration, target concentration or time period and press **Calculate**.

Time Unit

Half-Life values in the AquaChem database are saved as hours, however, you may convert these to days or years by selecting the appropriate **Time Unit** from the combo box.

Problem Type

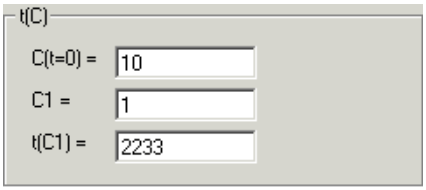
In the next line, you must specify the **Problem Type** for the degradation calculator. The Decay calculator has two problem types available:

Type 1: **Time to reach a specified concentration**; or
Type 2: **Concentration after a specified amount of time**

NOTE: If problem type 1 is selected, and the current contaminant has an assigned guideline level in your AquaChem database, a combo box with available guideline levels will appear to the right of the target concentration field. You have the option to choose the desired guideline level, and the **C1** value will be automatically filled in for you.

A summary of the required data input is as follows:

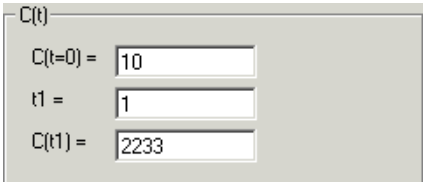
Problem Type 1:
Determine the time required for a contaminant to decay to a specified concentration



C(t=0): initial concentration
C1: target concentration

Press **[Calculate]** and the **t(C1)** (time to reach target concentration) will be calculated.

Problem Type 2:
Determine the concentration after a specified amount of time:



C(t=0): initial concentration
t1: target time duration

Press **[Calculate]** and the **C(t1)** (concentration after a specified time) will be calculated.

This calculator accounts only for degradation effect, using the following equation:

$C(t) = C1*e^{-kt}$

where,

k = residence time

Other effects such as dilution, transport, etc. are not taken into account with this tool. The **Aquachem.mdb** database currently contains degradations rates for approximately 90 contaminants. Other user-defined half-lifes may be entered for those chemicals not available in the database.

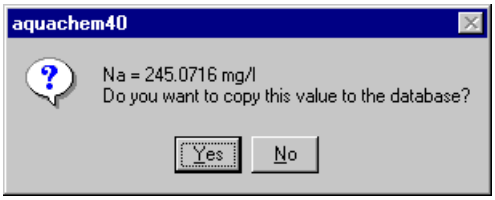
A complete set of degradation rates can be found in the following reference: Howard, P.H. et. al. 1991. *Handbook of Environmental Degradation Rates,* Lewis Publishers, 775 p. 1991

6.1.3 Find Missing Major Ion

If information for one of the major anions or cations (Na, Ca, Mg, Cl, HCO3, SO4) is missing from a sample, you can use this tool to estimate the concentration of the missing major ion. The concentration of the missing ion is calculated using the theoretical ion balance between the major ions.

NOTE: This tool is only available when you have a Sample Details window open and active.

Open a sample, and select **Tools > Calculators > Find Missing Major Ion > Na** (for the example shown below).



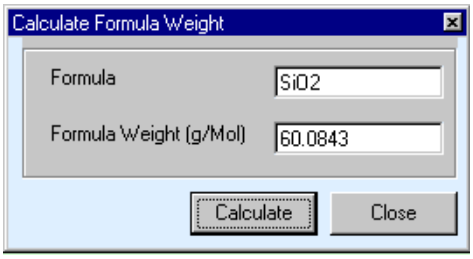
After you have selected the desired missing parameter, AquaChem will calculate the missing value and display a confirmation message as shown on the right. Click **[Yes]** to accept the calculated value, or click **[No]** to reject the calculated value.

This tool does not work if more than one of the major cations or anions is missing in the analysis. In order to calculate the missing values for one of the major ions, each of the remaining major ions must be present.

6.1.4 Formula Weight Calculator

This tool allows you to quickly calculate formula weights for a user-specified chemical formula.

When you access this tool, the **Calculate Formula Weight** dialogue will appear. Simply enter the desired formula, and press **[Calculate]**.

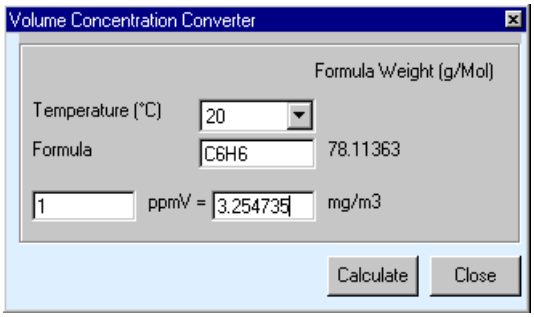


Note that the **Formula** is case sensitive; therefore, ensure that you enter Silicon as Si and not SI. In addition, only one level of parentheses is taken into account. So, in case of a formula with two levels of parenthesis such as ((XY2)3)3AC, it will not be calculated correctly.

6.1.5 Volume Concentration Converter

This converter allows you to quickly convert volume concentrations into mass concentrations for organic chemicals.

When you access this tool, the **Volume Concentration Converter** dialogue will appear. Simply choose the observed ambient **Temperature** (0, 20, or 25^{o}C), enter a **Formula** for an organic chemical, and enter the concentration. You may enter the concentration in either the **ppmV** or the **mg/m3** field.



Press **[Calculate]** and the missing concentration will be calculated.

In the vapor phase, one ppm by volume (ppmV) is on a volume per volume bases. For example, one ppmV of Benzene in the air means one part volume of benzene in one million parts volume of air space. To convert the ppmV into mass concentration units (mg/m3), the following formula can be used:

1 ppmV = FMW/K

where,

FMW = Formula Weight (g/mol)
K = is a temperature dependant coefficient (molar gas volume).

K= 22.4 l/mol at 0°C,
K= 24.05 l/mol at 20°C, and
K= 24.5 l/mol at 25°C.

Example:

To convert 1ppmV Benzene to mg/m3 at 20^{o}C:

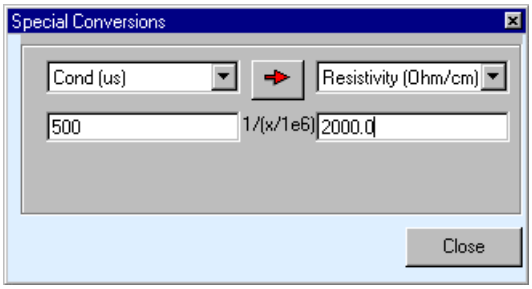
Mass Benzene mg/m3 = 1ppmV Benzene * [(78 g/mol) / (24.05 l/mol)]
= 3.24 g/L
= 3.24 mg/m3

Note that the Formula is case sensitive; therefore, ensure that you enter Silicon as Si and not SI. In addition, only one level of parentheses is taken into account (i.e. a formula such as ((XY2)3)3AC will not be calculated correctly).

6.1.6 Special Conversions

This tool provides conversions for numerous non-linear geochemical calculations. You may convert values from one measurement unit to another for measurement units such as pe - Eh, Alkalinity - HCO3, and Conductivity (us) - Resistivity (Ohm/cm).

When you access this tool, the **Special Conversions** dialogue will appear. Click on the button and choose a category from the list, enter the start value, and any other required variables (temperature, density), and press to convert the value.



The available conversion categories include:

Conductivity Resistivity

where,

Cond =1/(Resistivity/1E+6)

Electrical conductivity at a different temperature: Cond(T1) Cond(T2).
It requires you to enter a conversion temperature. The conductivity is always normalized to a specific temperature which is dependant on the probe. If you want to enter conductivity data to your database, and the temperature for the probe is different

(eg. 25°C) from the one in the database (20°C) then the data has to be converted before being adding to the database.

This calculation is done in two steps:

- First, calculate the conductivity at standard temperature,
- Second, calculate the conductivity at the specified temperature (Temp2).

Examples:

Cond.

Cond(25) = Cond(Temp1) / (1 + 0.0198 * (Temp1 - 25))
Cond(Temp2) = Cond(25) * (1 + 0.0198 * (Temp2 - 25))

Redox potential.

pe  Eh

It requires you to enter an observation temperature.

pe(Eh): pe = Eh * F / 2.303 / R / T
Eh(pe): Eh = pe * 2.303 * RT / F

where,

R = 8.314 (Gas constant)
F = 96485 (Faraday constant)

Reference: C.A.J. Appelo, 1996: *Geochemistry, Groundwater and Pollution, Balkema Roterdam, p. 246.*

Alkalinity calculations:

Convert between; mg/L HCO3,
mmol/L ,
Alkalinity (f*), where * means French degrees,
Alkalinity (g*), where * means German degrees mg/L CaCO3.

Reference: John D. Hem. *Study and Interpretation of the Chemical Characteristics of Natural Water,* USGS Water supply paper 2254, p. 158.

ppm  mg/L: Requires you to enter a density.

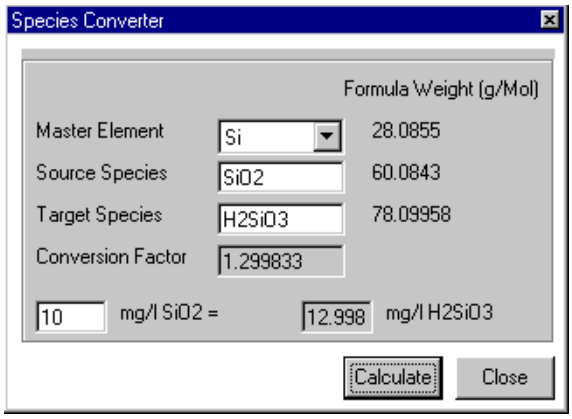
mg/L  ppm:
ppm = mg/L * density

ppm  mg/L:
mg/L = ppm / density

6.1.7 Species Converter

This tool allows you to convert any species into a different form.

When you access this tool, the **Species Converter** dialogue will appear as shown below:



- Select a **Master Element** (Parameter) for which you are interested in (common examples include phosphorus, silica, etc.).
- Type in a **Source Species**.
- Type in a **Target Species**.
- Enter a concentration of the source species in the lower left corner of the dialogue.
- The **Conversion Factor** is calculated based on the formula weights of the two species: the **Target species** divided by the **Source Species**.
- Press **[Calculate]** and the concentration for the target species will be calculated.

This tool is practical for expressing a measured amount of a parameter as different aqueous species when expressed in mg/L. For example, you may receive your Silica results as mg/L Si, and your database requires mg/L SiO2 or H2SiO3. For this you need to calculate the amount of SiO2 that holds the same amount of Silica as given in the lab analysis.

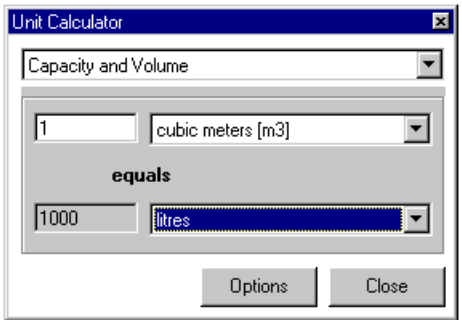
The data entered in the **Species Converter** dialogue (shown above) depicts an example for converting Si species.

Note again that the Formula is case sensitive; therefore, ensure that you enter Silicon as Si and not SI. In addition, only one level of parentheses is taken into account (i.e. a formula such as ((XY2)3)3AC will not be calculated correctly).

6.1.8 Unit Calculator

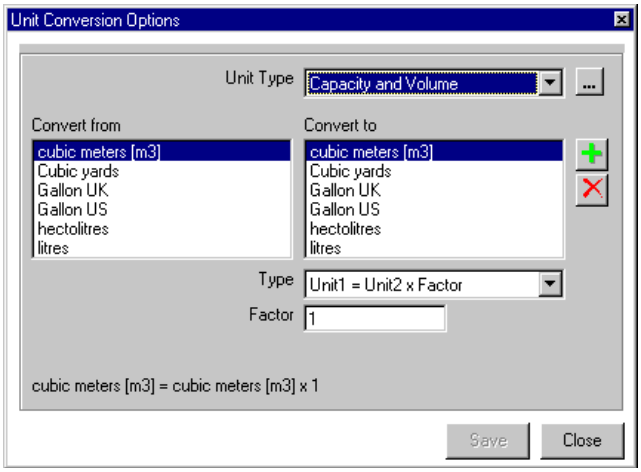
This tool performs basic unit conversions for length, time, volume, density, mass, etc.

When you access this tool, the **Unit Calculator** dialogue will appear as shown below.



Click on the button and select the desired category from the combo box at the top of the dialogue, enter the value and units in the fields below, and the new value will be automatically calculated.

In addition, you can modify the existing conversion factors, or create new ones. Press the **[Options]** button, and the following dialogue will be loaded.



Select the **Unit Type** from the combo list (at the top), or press the ... button to load a list of available unit types, and options to create a new unit type. The list below will now show all conversions available for this unit type, and the conversion factor associated with each. You may enter or edit all factors, or create new conversions using the button. Then enter the appropriate conversion type and factor for this new conversion.

Once you are finished, press **[Save]** to save any changes you made to the conversions.

Press **[Close]** to return to the **Unit Calculator** tool.

6.2 LookUp Tables

The Look-Up Tables menu displays the available AquaChem tables containing useful hydrochemical information. Look-Up tables allow you to store and retrieve any useful information from within the Aquachem environment. The tables are created using MS Access, and are saved in the Aquachem.mdb database. These new tables can then be displayed and searched in Aquachem.

The first three tables are used by AquaChem for internal calculations, and can not be modified.

- Degradation Rates
- PHREEQC Phases
- Periodic Table

The remaining table is an example of user-defined table:

- Adsorption Isotherms

These tables can be modified by selecting **File** from the main menu and then **Database**. These tables are used for lookup purpose only, and are read-only. You may create up to ten user-defined tables. All other tables may be defined, provided you have MS Access2000 development environment.

The **Demo** database includes one example Look Up Table, which is meant for demonstration purposes only and do not represent a complete dataset. This provides an example of useful data which can be used in an AquaChem project. You may create your own tables which may be used for a specific study, and bring these tables into AquaChem.

For more details on creating user-specified LookUp tables in AquaChem, please refer to the Lookup Tables in Chapter 3.

6.2.1 Degradation Rates

This table provides a list of **Degradation Rates** for organic compounds. Half-life values are available for various phases (Soil, Air, Surface water, and Groundwater). All

half-life values are displayed in hours. The data from this table is used for the **Decay Calculator**. These degradation rates are from the following reference:

Howard, P.H. et. al. 1991. *Handbook of Environmental Degradation Rates*, Lewis Publishers, 775 p.

6.2.2 PHREEQC Phases

The minerals list is read from the PHREEQC thermodynamic database file. If no valid thermodynamic database is specified, the **List of Minerals** will be empty. This table displays PHREEQC phase names, formula, and molecular weights.

6.2.3 Periodic Table

This tables provides information for all elements in the **Periodic Table**. This includes: Name, Formula, Mass, Valence, CAS #, and Group Name.

6.2.4 Adsorption Isotherms

This table includes details on adsorption parameters for several chemicals.

6.3 Modeling

The **Modeling** option under the **Tools** menu provides links to the PHREEQC geochemical modeling utilities.

PHREEQC provides five options for geochemical calculations:

Option 1: Calculation of the aqueous equilibrium (activities and saturation indices) based on a sample analysis
Option 2: Calculate pH based on a sample analysis
Option 3: Calculate Eh based on a sample analysis
Option 4: Basic forward modeling, such as mixing samples, adding minerals or chemicals to a solution, or raising temperature
Option 5: Advanced modeling such as transport calculations, inverse modeling, etc.

Option 1

AquaChem allows you to quickly calculate saturation indices and activities for the modeled parameters listed in your database; the results are automatically saved back to your database, provided that the fields exist in the database. For example, to read back the calcite saturation index calculation, you need a field SI_Calcite specified in the **Database Options**, **Modeled Parameters** section.

Option 2

AquaChem allows you to use PHREEQC to calculate a pH value for your sample. This can be used in an instance where you do not have a pH value for your sample, or you would like to compare the measured pH value to the modeled value.

Option 3

AquaChem allows you to use PHREEQC to calculate the Eh value for your sample. The calculation is based on the available redox couples for the selected sample.

Option 4

Aquachem also allows you to do basic modeling with the PHREEQC interface included with AquaChem. To do so, you must use the **PHREEQC (Basic)** option. This option allows you to create input files, and run simulations which include basic forward modeling, such as mixing samples, adding minerals or chemicals to a solution, etc. PHREEQC input files may contain samples from your AquaChem database or a Pure Water solutions. Before creating a PHREEQC Input file, it is recommended that you have some basic knowledge about PHREEQC. For more details, please refer to the PHREEQC User's manual which is included with your AquaChem installation.

Option 5

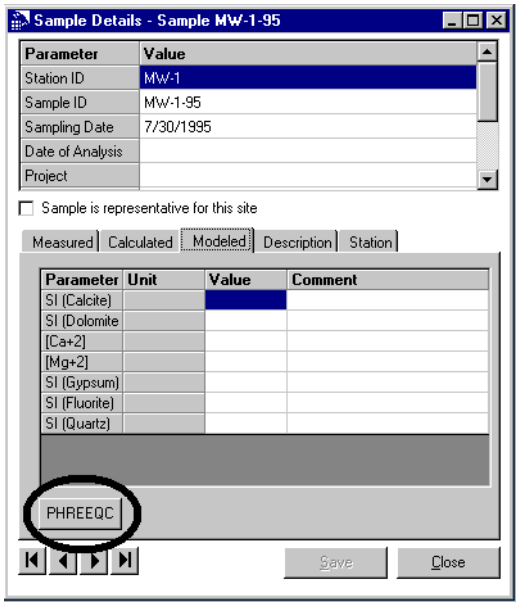
For a more advanced simulation, AquaChem provides links to the two versions of PHREEQC which are distributed by the USGS: PHREEQC-I and PHREEQC for Windows. These versions offer the full features of PHREEQC, including transport, inverse modeling, and kinetics. In order to do advanced modeling, and exploit all the features of PHREEQC, it is encouraged that you use one of these versions of PHREEQC.

You may link either one of the mentioned programs to Aquachem in the **File > Preferences** and launch this program through the **Tools > Modeling > PHREEQC (Advanced)** menu option. When this program is launched, an input file will be created automatically, and will contain any selected sample(s) from your Aquachem active samples list. Alternatively, you may create a new, empty, input file.

6.3.1 Calculate Saturation Indices and Activities

When you select this item from the **Tools > Modeling** menu, PHREEQC will run for each selected sample, and calculate saturation indices and activities for all modeled parameters which are defined in the current database structure. The results of the simulation will be automatically written back to the database for each selected sample, provided that the fields exist in the database. For example, to read back the calcite saturation index calculation, you need a field SI_Calcite specified in the **Database Options**, **Modeled Parameters** section.

If you would like to calculate Saturation Indices (SI) or activities for **one** sample in your database, simply load the appropriate Sample Details window, then click on the Modeled Parameters tab. Once you have done this, click on the PHREEQC button, which is located in the lower left corner of this window (as circled below):

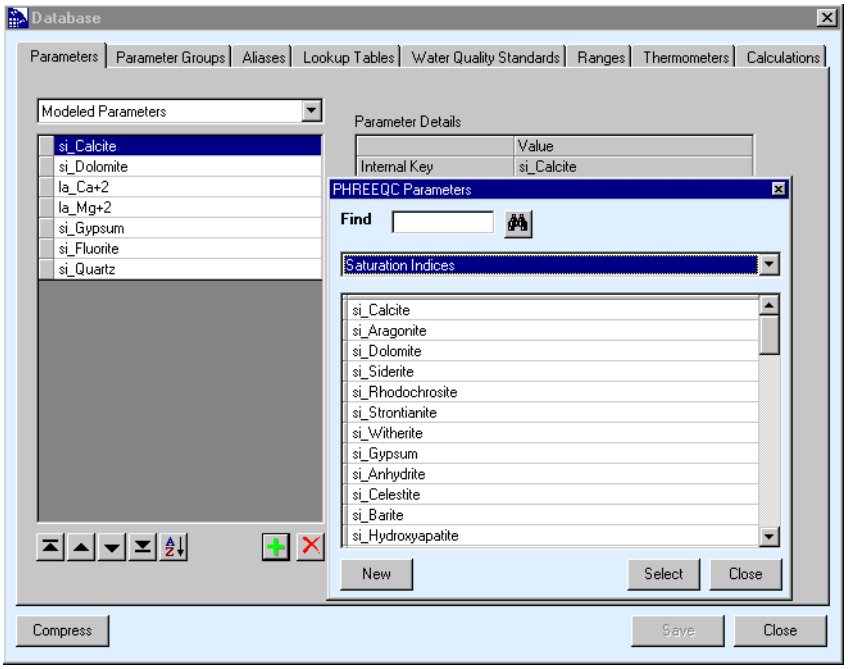


PHREEQC will then run in the background, and the modeled results will be saved automatically back to your database. There is no need to create and define input files.

If you would like to quickly calculate Saturation Indices (SI) or activities for **multiple** samples in your database, then you should use the **Calculate Saturation Indices and Activities** menu option. When this option is selected, PHREEQC will run once for each sample which is selected in the active list window. The modeled results will be saved automatically back to your database, for each selected sample.

To add additional modeled parameters to your database structure, you must load the Database options, under **File > Database > Parameters**. Then, select the **Modeled**

Parameters from the combo box, and add the desired Saturation Indices and Activities to your database (as shown in the dialogue below).



An example of how to **Calculate Saturation Indices and Activities** is provided below:

Example

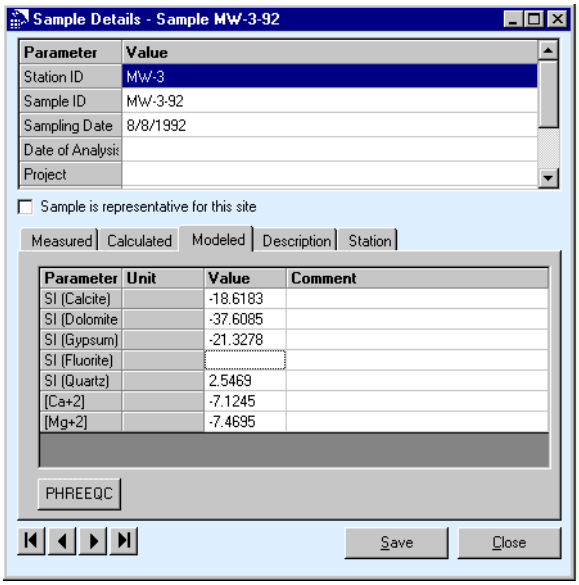
To model a sample from the **Demo.AQC** database:

- ☞ Select any sample from your Active Samples List.
- ☞ **Calculate Saturation Indices and Activities** from the **Tools > Modeling** menu.

You will then see a PHREEQC DOS window run in the background. Once this is finished, load the Sample Details window for this sample, then

- ☞ **Modeled** Parameters tab

In this window, you will see the modeled values for the available parameters. An example is shown in the figure below:



You may now do further processing and analysis with these parameter values, such as plotting, reporting, and querying.

6.3.2 Calculate pH

This tool can be used to estimate a missing pH value for an individual sample. The pH is calculated, based on the assumption that the groundwater comes from a carbonaceous aquifer and is in equilibrium with calcite. Usually a saturation index (SI) of 0 is thus specified. If a different SI is knows for samples in the region, a different value can be specified.

Alternatively, if a pH value was measured, and again the groundwater is assumed to be in close equilibrium with calcite, this tool can be used to test at which value the pH would be if the hypothesis was true, or to validate the measured pH value.

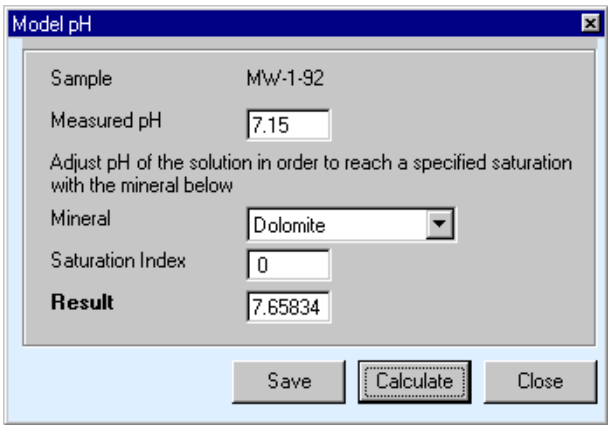
An example is provided below.

Example

To model the pH for a sample from the **Demo.AQC** database:

- Select any sample from your Active Samples List.
- **Calculate pH** from the **Tools > Modeling** menu.

You will then see the following dialogue:



The **Sample** and **Measured pH** will be filled in automatically.

- ☞ Select a **Mineral** from the combo box.
- ☞ Enter a value for the **Saturation Index** for this Mineral. This may be from a previous simulation, or other know values.
- ☞ **[Calculate]**

You will then see a PHREEQC DOS window run in the background. Once this is finished, a calculated pH value will appear in the **Result** field.

To accept this calculated pH value,

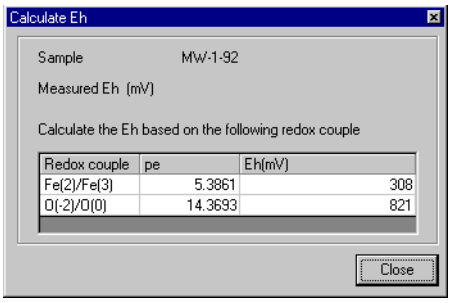
- ☞ **[Save]**

Otherwise,

- ☞ **[Close]** to return to the main window.

6.3.3 Calculate Eh

In some cases, it may be very difficult to obtain meaningful Eh values by direct measurements. Several authors have recommended to calculate the Eh by means of the redox speciation with the Nernst Equation. Each Redox couple, e.g. Fe2+/Fe3+, Mn2+/Mn3+ gives an individual Eh value, which in cases of equilibrium conditions, should be reasonable. The **Calculate Eh** menu item launches PHREEQC to search the selected sample for available redox couples and to calculate pe and Eh values for each couple. A sample of the dialog is shown below:

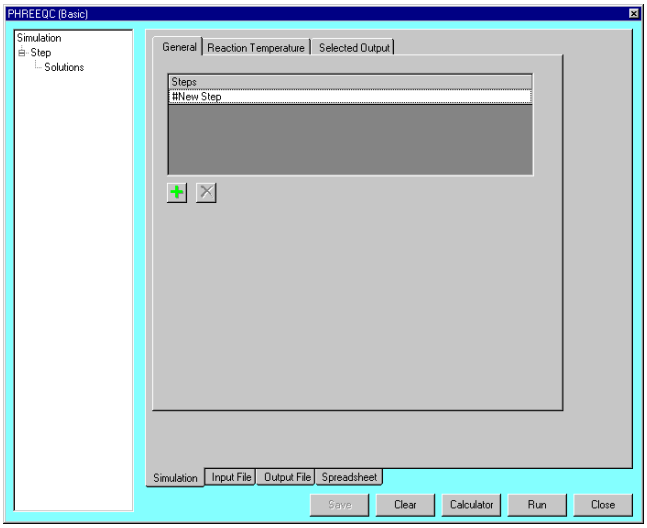


The calculated Eh value may be compared to your measured Eh value.

In order to use this modeling utility, you must have data entered for a minimum of 1 redox couple (ex. Fe2+ / Fe3+), in the sample details window, **Measured** parameters tab.

6.3.4 PHREEQC (Basic)

This option loads the **PHREEQC (Basic) Input file** dialogue as shown below.



The AquaChem PHREEQC interface allows you quickly and easily create input files for running simple PHREEQC simulations in a Windows environment. This unique graphical environment facilitates rapid development of simple PHREEQC simulations. Only the basic features of PHREEQC are supported; to take advantage of the more advanced features (Inverse Modeling, Transport, and Kinetics), you may utilize one of the USGS's PHREEQC versions, as explained below.

AquaChem provides direct access to your AquaChem project database samples for selecting solutions and building the input files. New solutions can be easily defined as needed, or existing solutions from previous simulations can be conveniently selected.

AquaChem also supports the use of flexible units for the various chemicals in solution.

Several simulations can be defined in one input file and processed in a single run. Reactions such as heating, evaporating, dissolving, or precipitating minerals can be conveniently simulated in step wise simulations, with all model parameters calculated for each step.

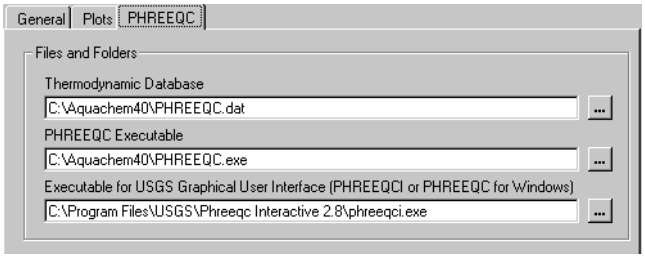
Once the PHREEQC input files have been prepared, the simulation can be launched directly from AquaChem. When the PHREEQC simulation is completed, you can copy the results from the spreadsheet view, and paste these into the Sample Details window for each individual sample. This will allow you to do further processing and analysis, such as plotting, reporting, and querying.

NOTE: Before using PHREEQC, you must ensure that you have defined the location of the PHREEQC.exe (executable), and PHREEQC.dat files. This can be done in the **PHREEQC Preferences** dialogue, available in the **File** menu.

For more details on designing a PHREEQC input file, please refer to Chapter 7: **GeoChemical Modeling with PHREEQC (Basic)**.

6.3.5 PHREEQC (Advanced)

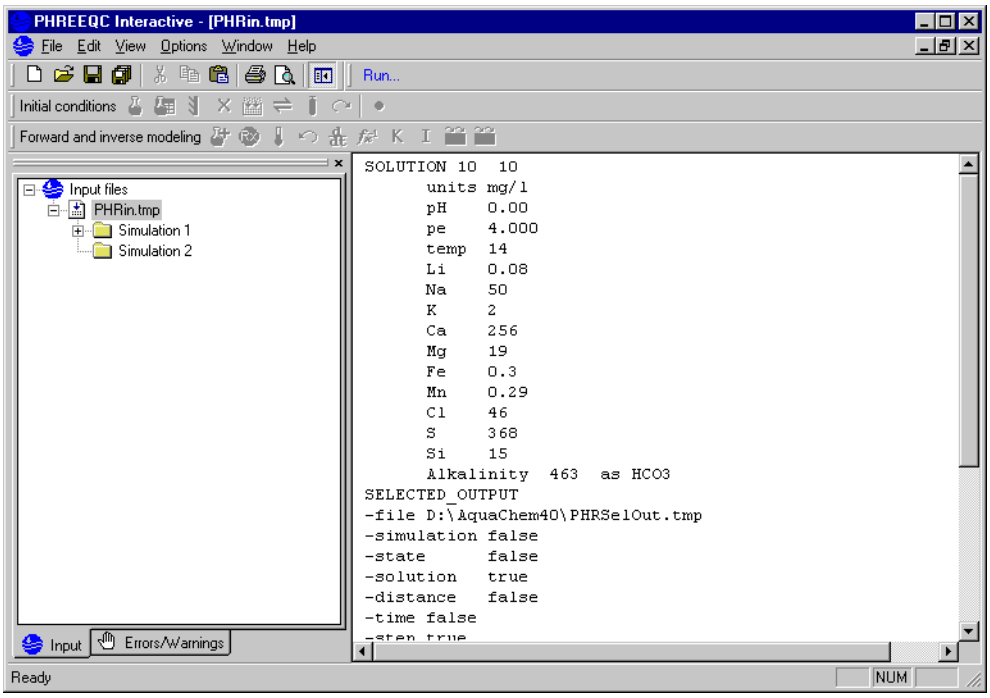
This option allows you to run advanced PHREEQC simulations, using either PHREEQC-Interactive or PHREEQC for Windows. The PHREEQC version that is loaded will be dependent upon the .exe file which is specifed in the Preferences dialogue, as shown below:



In the third line under **Files and Folders**, you will see a field where you can specify the location of the PHREEQC executable file. If you are using PHREEQC-I, the file is called **phreeqci.exe**. If you are using PHREEQC for Windows, the file is called **phreeqc.exe**. Please point this to the appropriate folder on your system where the respective installation resides.

PHREEQC-Interactive

When you select the PHREEQC (Advanced) option from the **Tools > Modeling** menu, this will load the USGS's PHREEQC- Interactive Windows Interface, provided that this component was successfully installed during your AquaChem installation. An example of the PHREEQC-I window is shown below:



Any sample(s) which are selected in your active list will be used as initial solutions when you load the PHREEQC-I program. You may select individual or multiple samples in your active samples list. From this point, you may then use the full features which PHREEQC-I has to offer. Once a PHREEQC-I simulation is completed, you must manually insert the results back into AquaChem by copy-and-paste, or by manual entry.

NOTE: Before using PHREEQC-I, you must ensure that you have defined the location of the PHREEQCI.exe (executable). This can be done in the **PHREEQC Preferences** dialogue, available in the **File** menu. If you did not install PHREEQC during your AquaChem installation, you may install this using the installation files located in the PHREEQC folder of your AquaChem CD-ROM. The installation file is named: PhreeqcI28.exe.

For more details on PHREEQC-I, please refer to the user's manual "manual.pdf" which can be found in the 'Doc' folder, in your PHREEQC-I installation directory. Or, you

may access the PHREEQC-I On-Line help, from within PHREEQC-I (in the Help menu).

PHREEQC for Windows

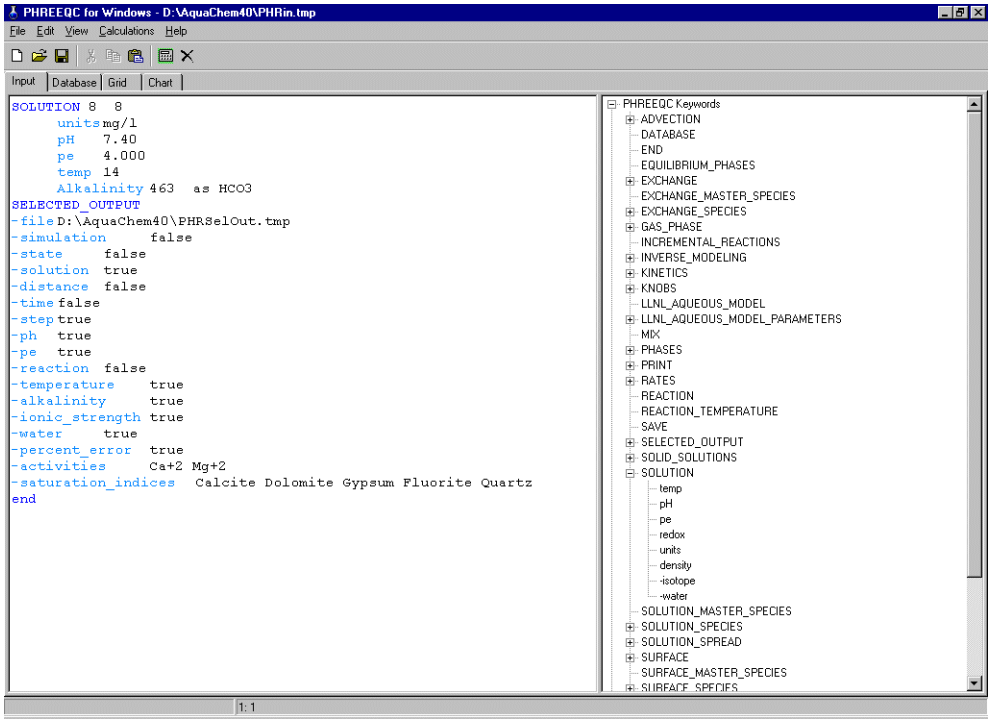
PHREEQC for Windows is a 32-bit Windows version of the geochemical model PHREEQC. PHREEQC for Windows contains the full functionality of PHREEQC v.2. The input files for the program are backward compatible with the normal version of PHREEQC. This means that you can use any file created with the normal version in PHREEQC for Windows. However, some options that are available in PHREEQC for Windows are not available in the standard version. The GUI for PHREEQC for Windows is developed by Vincent E.A. Post.

PHREEQC for Windows is not included with the AquaChem installation. If you would like to install this program, you may use the installation files which can be found on your AquaChem CD-ROM, in the PHREEQC folder. The installation file is named **psetup1510.exe**. PHREEQC for Windows is a freeware product, and may be downloaded from the website below:

http://www.geo.vu.nl/users/posv/phreeqc.html

Once you have installed PHREEQC for Windows, you must define the location of the PHREEQC.exe (executable), in the **PHREEQC Preferences** dialogue, available in the **File** menu. Then, this executable will be launched when you select **PHREEQC (Advanced)** from the **Tools > Modeling** menu option.

An example of the input window for PHREEQC for Windows is shown below:



Similar to the PHREEQC-I, any sample(s) which are selected in your active list will be used as initial solutions when you load the PHREEQC for Windows program. You may select individual or multiple samples in your active samples list. From this point, you may then use the full features which PHREEQC for Windows has to offer. Once a simulation is completed, you must manually insert the results back into AquaChem by copy-and-paste, or by manual entry.

For more details on PHREEQC for Windows, please refer to the user's manual "ManualW.pdf", which can be found in your PHREEQC for Windows installation folder. Or, you may access the On-Line help, from within PHREEQC for Windows (in the Help menu).

7

GeoChemical Modeling with PHREEQC (Basic)

This chapter presents an overview of the modeling capabilities of PHREEQC, an introduction on how to Create PHREEQC Input files and visualize output using the basic version of PHREEQC included within the AquaChem interface.

There will be an introduction to the AquaChem Interface to PHREEQC, PHREEQC Window Layout, Creating PHREEQC Input Files, Running PHREEQC Simulation, as well as Viewing PHREEQC Output.

For details on PHREEQC-I, or PHREEQC for Windows, please refer to the User's Manuals included with these programs. Or, for a basic description, please refer to Chapter 6: **PHREEQC (Advanced)**.

7.1 AquaChem Interface to PHREEQC

PHREEQC is a computer program for speciation, batch-reaction, one-dimensional transport, inverse geochemical calculations, and much more. For more than twenty years, the USGS's PHREEQC has been the proven standard for aqueous geochemical modeling. PHREEQC is derived from the FORTRAN program PHREEQE. As the name implies, the original FORTRAN code has been entirely rewritten in the C programming language and this new version has eliminated many of the deficiencies and limitations of earlier version of PHREEQE, while adding many new powerful analytical capabilities.

In the past years the authors of PHREEQC have not only added many more powerful features to the program, but they have also implemented two very easy-to-use interfaces for writing input files and analyzing output files for the PHREEQC program. The respective programs PHREEQC-I and PHREEQC for Windows are included with your AquaChem installation CD; you may link your AquaChem samples in your database to either one of these programs, provided that these programs are installed, and linked in the **File > Preferences** dialogue. These interfaces may be called from

within AquaChem, and this will allow you to run advanced PHREEQC simulations using your AquaChem samples. For more details, please refer to Chapter 6.

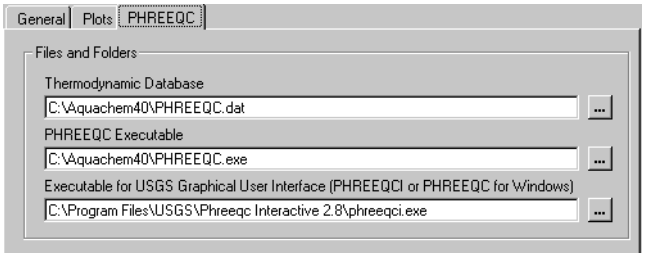
The PHREEQC (Basic) option provides a GUI to the basic features of PHREEQC. You may run simple simulations by integrating your AquaChem samples; this option also allows you to create input files, which can be integrated with the more advanced versions of PHREEQC, allowing for a complete integration between your AquaChem water sample data, and geochemical simulations with PHREEQC.

Although this chapter describes how to create PHREEQC input files with the PHREEQC (Basic) version, the concept of hydrochemical modeling and the PHREEQC program will not be discussed in detail. It is recommended that you read the PHREEQC user's manual before performing any complex hydrochemical simulations. For your reference, the PHREEQC user's manual and source code may be downloaded from the following web site: http://water.usgs.gov/software/geochemical.html. In addition, the PHREEQC user's manual is available on the AquaChem installation CD-ROM, and in your AquaChem installation folder.

7.1.1 Preferences for PHREEQC

The instructions in this chapter will be based on the assumption that you are using the PHREEQC executable file (PHREEQC.exe - PHREEQC version 2.8) included with AquaChem v 4.0. By default, the PHREEQC executable file and the PHREEQC thermodynamic database files are automatically installed in the default folder, C:\AquaChem40. If you have installed AquaChem in a directory other than the default installation directory, you will need to manually set up the link between AquaChem and the PHREEQC thermodynamic database and executable files.

To do so, select **File** from the main menu and then select **Preferences**. The following **Preferences** dialogue will appear. In this dialogue, select the **PHREEQC** tab.



Under the **Files and Folders** frame, press ... button beside the **Thermodynamic Database** field and select the path and filename from the **PHREEQC Thermodynamic**

Database dialogue. From this dialogue, select either **phreeqc.dat**, **Wateq4f.dat** or **Minteq.dat**. In addition, in the **PHREEQC Executable** field select the path and filename for the **phreeqc.exe** file. Finally, specify the path and filename for the USGS PHREEQC Executable file (which is used in the PHREEQC (Advanced) option). If the default path and filename are incorrect, you can browse the directory by clicking on the  button and select the filename.

By default, all PHREEQC input and output files will be saved in your AquaChem installation folder (default is C:\AquaChem40).

Once you are finished, click **[Save]** then **[Close]**. You are now ready to run PHREEQC.

7.1.2 The PHREEQC Thermodynamic Database Link

One of the biggest advantages of the AquaChem PHREEQC interface is the direct link between the two databases of these programs. The link allows you to use samples from the AquaChem database and read them into the PHREEQC input data file.

In order to let AquaChem know which database parameter corresponds to which PHREEQC element, some minor modifications have been made to each of the thermodynamic databases included with AquaChem. The link between AquaChem and the thermodynamic databases is established by adding the AquaChem parameter name as a comment for each matching parameter in the Masterspecies section of the database file. Each comment is preceded by a '#' character to flag the AquaChem parameter descriptor.

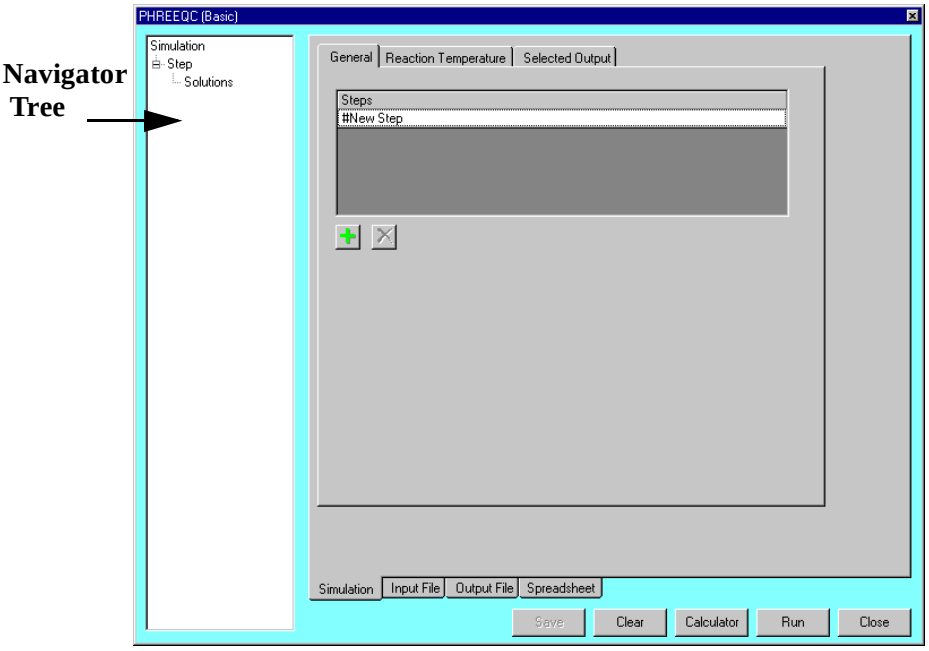
For example, the following lines are taken from the Masterspecies section of the **phreeqc.dat** file:

Ca	Ca+2	0.0	Ca	40.08	#CA
Mg	Mg+2	0.0	Mg	24.312	#MG
Na	Na+	0.0	Na	22.9898	#NA
K	K+	0.0	K	39.102	#K
Fe	Fe+2	0.0	Fe	55.847	#FE
Fe(+2)	Fe+2	0.0	Fe		
Fe(+3)	Fe+3	-2.0	Fe		
Mn	Mn+2	0.0	Mn	54.938	#MN

These modifications have already been defined for each of the thermodynamic database files provided with AquaChem. You have to redefine this only if you change the thermodynamic database.

7.2 PHREEQC Window Layout

To access the PHREEQC input dialogue, select **Tools** from the main menu of AquaChem and **Modeling** and then **PHREEQC (Basic)**. This will load the **PHREEQC (Basic) Input** dialogue as shown in the following figure.



The **PHREEQC Input** dialogue consists of several options and settings that apply to the entire PHREEQC simulation.

The left side of the dialogue includes a **Navigator Tree**, allowing you to quickly add and modify the reaction options for the current simulation.

Along the lower part of the **PHREEQC Input** dialogue there are four tabs:

Simulation This allows you to define the simulation options (main input dialogue).

Input File This provides a view of the PHREEQC input file, in text format.

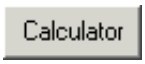
Output File This provides a view of the PHREEQC output file, in text format.

Spreadsheet This provides a spreadsheet preview of the PHREEQC output file.

The bottom of the **PHREEQC Input** dialogue contains several buttons:

The save button allows you to save the contents of the input or output file. If the **Input File** tab is selected, the Save button will allow you to save the input file as a .**PQI** file. If desired, this file may be loaded into PHREEQC-I, and the simulation may be run using this version. If the **Output File** tab is selected, the Save button will allow you to save the output file as a .**PQO** file.

The clear button clears the contents of the input file, and allows you to create a clean, new input file.

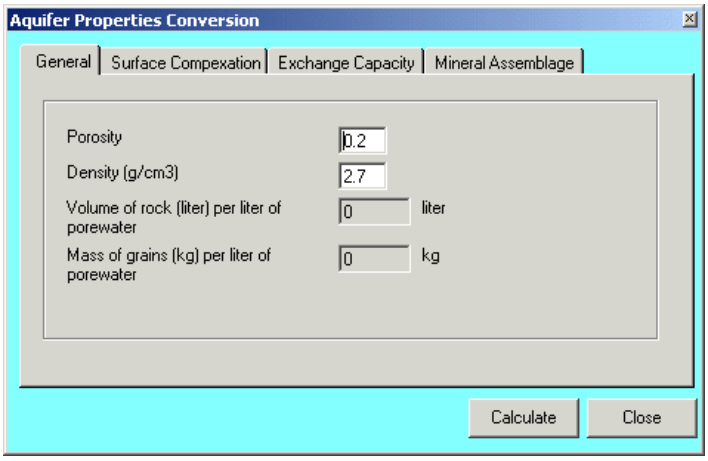


The Calculator button loads the **Aquifer Properties Conversion** dialogue and allows you to calculate the various aquifer properties you require for some of the PHREEQC simulations.

The Close button closes the PHREEQC input dialogue.

The Run button runs PHREEQC using the current simulation options. This button loads the PHREEQC input file and executes the PHREEQC simulation. The **[Run]** button should only be used after you have specified all of the required run options and you are ready to start the PHREEQC simulation. It is recommended that you verify the input file before running the simulation.

There are four tabs associated with the **[Calculator]** button: **General**, **Surface Complexation, Exchange Capacity,** and **Mineral Assemblage**. These are shown and described below:

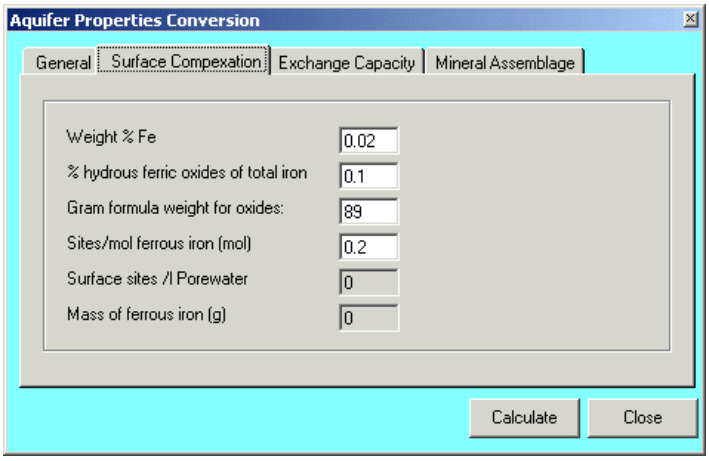


General

Since PHREEQC always assumes a solution volume of 1.0 liters, the **General** calculator allows you to easily calculate the **Volume of rock (liters) per liter of porewater** and **Mass of grains (kg) per liter of porewater** for the aquifer based on a solution containing 1.0 liters of porewater. Simply enter the input parameters (**Porosity**, **Density**), and press the **[Calculate]** button.

Surface Complexation

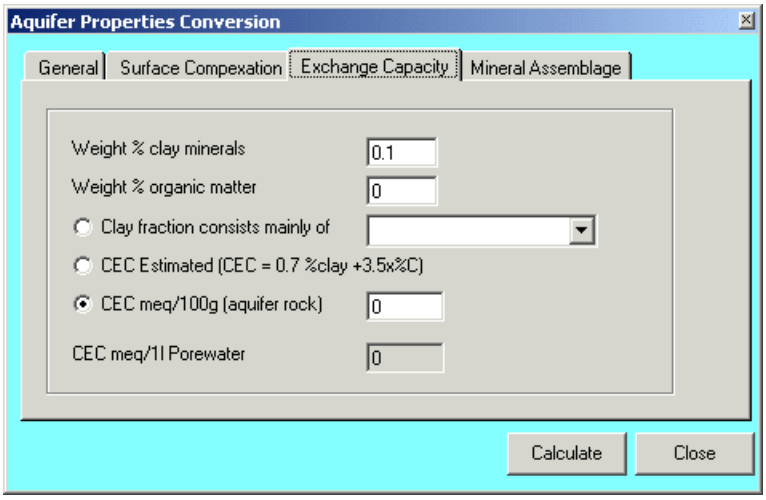
The moles of surface places (**sites**) depends on the content of hydrous ferric oxides in the aquifer (**Sites/mol ferrous iron**). **Fe** is generally a measured parameter but you must estimate the percentage of iron (**Weight % Fe**) that is in the form of hydrous iron (**% hydrous ferric oxides of total iron**). Since PHREEQC always asks for mols, you also need a formula weight value for your iron minerals. Hydrous iron is a mixture of several minerals, so a suggested **Gram formula weight for oxides** is **89** which is used as a default value.



Exchange Capacity

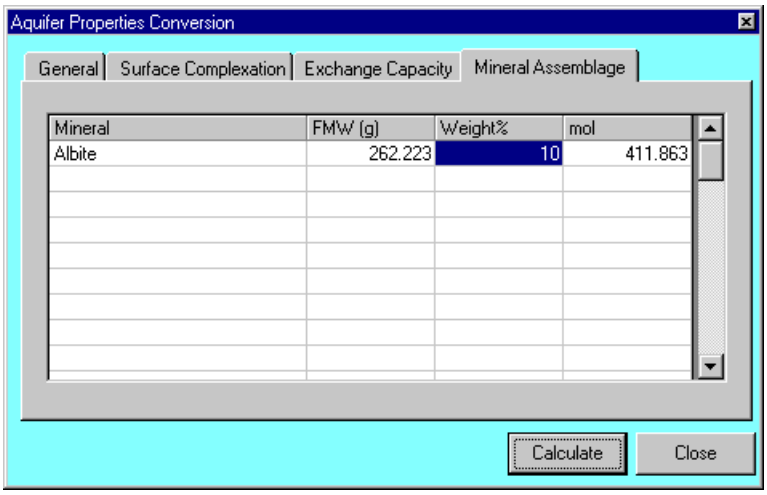
The Cation Exchange Capacity (CEC) is normally expressed as meq/100g. If you know this value you may directly enter it and calculate the exchange places (**Sites**) within the given aquifer volume. Otherwise you need to estimate the CEC. The first option lets you select a clay mineral from a list and will use an average CEC value. Choose this option if know the dominant clay mineral of your aquifer. If you know only the percentage but not the mineralogy of your clay minerals you may use a formula derived by Appelo (1993) to estimate the CEC:

CEC=0.7 * clay% +3.5 * org material%.



Mineral Assemblage

The Mineral Assemblage option lets you convert an analysis expressed as weight percent to mmol/l porewater. Simply select a mineral from the combo box, and specify a Weight %. Press **[Calculate]** and the amount of mols will be calculated.



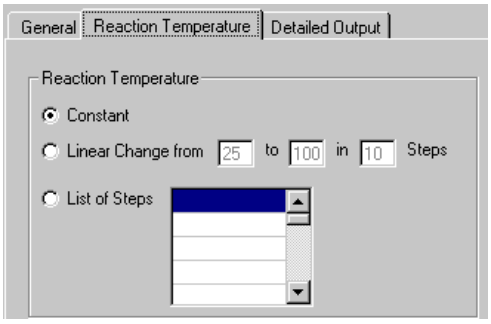
There are three tabs associated with the **Simulation** tab which are shown and described below:

General

The **General** tab contains a summary of the steps defined for the current simulation.

Reaction Temperature

This tab provides options to specify the reaction temperature, or step-wise changes in the reaction temperature. The **Reaction Temperature** options can be seen in the dialogue shown below.

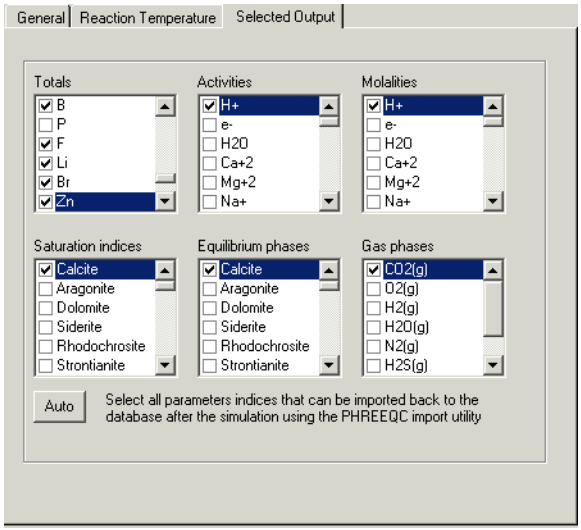


The **Reaction Temperature** tab provides options for specifying the desired temperature settings. Normally the temperature of the selected sample stays **Constant** (default setting) during a reaction and it will use the solution temperature as entered in the **Solutions** option selected from **Navigator tree**. However, PHREEQC provides you the options to change the temperature linearly (**Linear change from...to...in...Steps)** from a starting temperature to an ending temperature in a specified number of steps or in steps during the course of a simulation. The **List of Steps** option allows you to specify the exact temperature at specific steps during the reaction and the temperatures will be applied in the order they are listed.

Selected Output

The **Selected Output** tab allows you to access the various output details to include in the standard PHREEQC results output file (**.PQO** file extension). PHREEQC will generate an output file every time you run a simulation. However, this file is very detailed and may contain more information than you need to solve a particular problem. This tab lets you create a customized simulation results file containing simulation data for only the parameters in which you are interested.

The options available under the **Selected Output** dialogue are shown in the figure below:



Simply choose the parameters you want to save to the tabular output file. By default the parameters **pH**, **pe**, **Temperature** and **Ionic Strength** are included in the output.

The Auto button will automatically select only the modeled parameters which you have defined in your database.

When you have successfully run the simulation, AquaChem allows you to save the output file. To do so, press the Save button, and enter a filename.

Save Options

The "**Save Solution as**" option in the step frames, allow you to save the current simulation and a defined name. You may afterwards continue to model with one of the USGS GUIs that provide more advanced coverage of the PHREEQC features.

7.3 Creating PHREEQC Input Files

The PHREEQC interface in AquaChem v. 4.0 has been re-designed to allow for more flexibility when creating and modifying input files. The following improvements have been made:

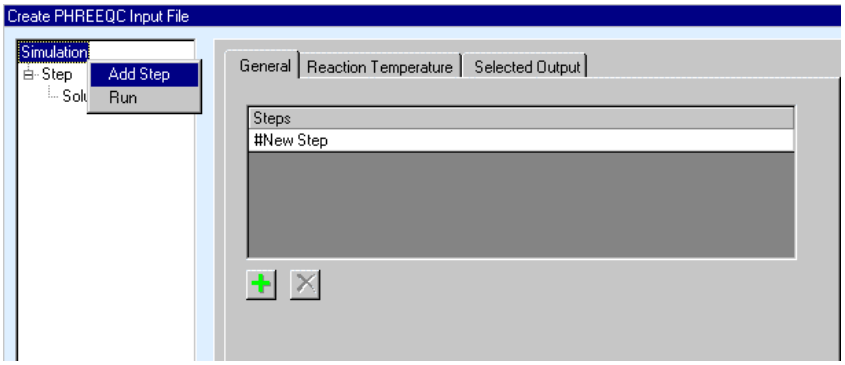
- The entire PHREEQC simulation is now saved to memory; this means that steps, solutions, and reactions will be added automatically to the input file, as they are selected.
- As shown above in the **PHREEQC Window Layout**, the input dialogue now contains a **Navigator tree** on the left side of your display, and a main input window on the right side of your display. This allows you to quickly navigate through the simulation options, and to make quick changes and re-run a simulation.

7.3.1 Simulation - Steps

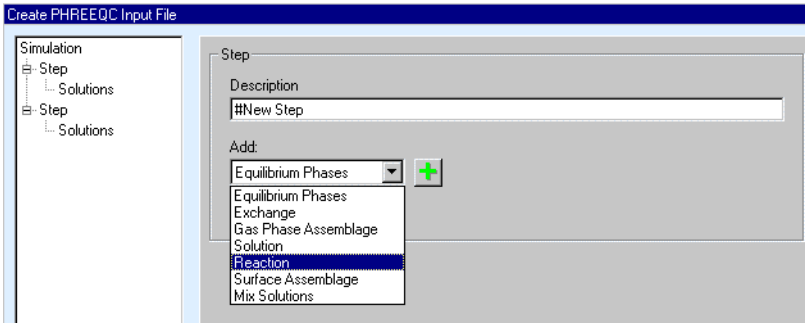
A PHREEQC simulation may consist of several steps. Each step must contain at least one solution.

Under the **General** tab, you will see a list of **Steps** (if multiple steps have been defined).

In order to add a simulation step you may right click on **Simulation** - the top item of the **Navigation tree** - and select the **Add Step**. Or click the  button below the **Steps** frame.



You can enter a name for the **Step** in the **Description** field, and choose the step properties. Click button under the **Add** and choose an item from the list, and press the  button.



This new item will now appear in the **Navigator tree** on the left side of your display. To activate the properties for this item, expand the **Navigator tree** and click once on this item.

To modify the **Step** properties, you have two options:

(1) Double click on the **Step** name from the main dialogue, OR
(2) Select "**Step**" from the **Navigator tree** on the left side of your display.

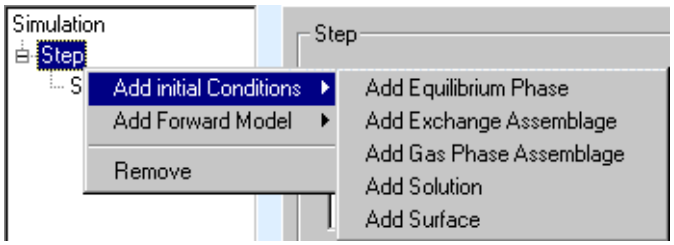
Options for the reaction steps can also be created and modified as needed. These include:

- **Add Initial Conditions** and
- **Forward Modeling**

These options are described in detail in the following sections.

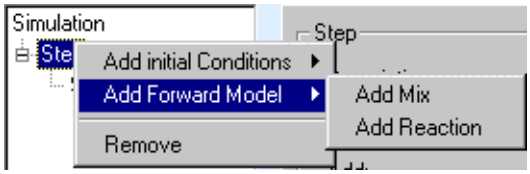
Add Initial Conditions

Add Equilibrium Phases
Add Exchange Assemblage
Add Gas Phase Assemblage
Add Solutions
Add Surface Assemblage



Forward Modeling

Add Mix Solutions
Add Reactions



7.3.2 Equilibrium Phases

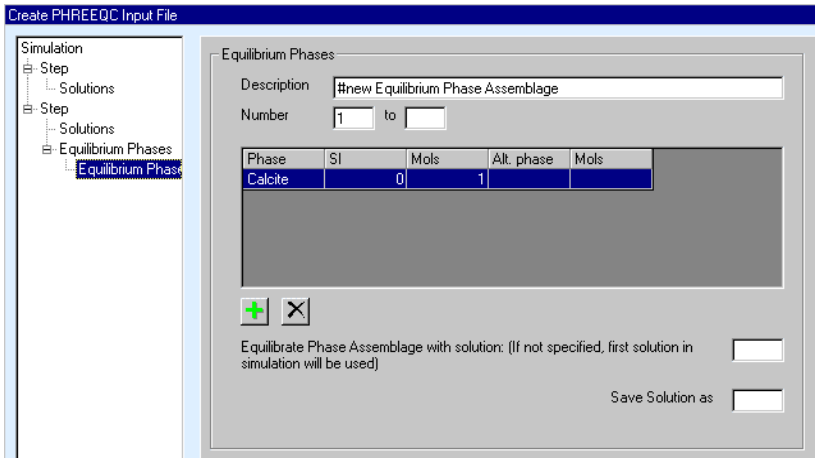
Adding Equilibrium mineral phases is similar to adding reactions. With the **Add Reaction** options (described below) you add a specified amount of a phase, but with the **Add Equilibrium Phase** options the amount of mineral phase added is limited by a specified saturation index.

To specify an equilibration of your solution with Mineral Phases, right click on the **Steps** options and select **Add Initial Conditions** from the popup menu and then select **Add Equilibrium Phases**.

Equilibrium Assemblage

Each mineral phase assemblage is identified by a unique **Phase** assemblage **Number** and a **Description**. You may enter multiple phases by specifying a phase number from # to # (ex. Number 1 to 2).

- Select **+** beside **Equilibrium Phases** (in the **Navigator tree**) and you will see **Equilibrium Phases1**
- Select **Equilibrium Phases1** and an **Equilibrium Phases** dialogue will appear as shown below.



For each mineral phase you choose, you can specify the following properties:

SI: This is the Saturation Index of the selected mineral phase (degree of saturation, default value 0).

$$SI = \log(IAP/KT)$$

where,

IAP = the ion activity product for the given material and
KT = the reaction constant at the given temperature

If SI > 0, then the solution is super-saturated with respect to the mineral phase;
If SI < 0, then the solution is below saturation of the specified mineral phase.
If SI = 0, then the solution is in equilibrium with the specified mineral phase.

For Gas phases the SI corresponds to the log of the partial pressure.

Mols: Mols describes the maximum amount of mineral phase that can be added or dissolved to reach the specified saturation. The default value is 10 mols. This value is typically used for transport problems in order to define a pure phase assemblage.

Alternative phase: The alternative phase is added or removed until the first mineral is in equilibrium with specified saturation index. For example, gypsum may be added or removed to the solution until an equilibrium with calcite is reached. An amount must be specified for the alternative mineral phase (default amount of the alternative phase is 10 moles as specified by PHREEQC). The solutions equilibration with calcite will be terminated if the amount specified for the alternative mineral phase is consumed prior to equilibration with calcite. It should be noted that if the alternative phase is specified,

the amount of the mineral phase must be equal to zero (i.e. it is not possible to have both an excess of the specified mineral phase and the alternative phase).

Below the grid, select the solution with which the mineral phase will be equilibrated. If you do not choose a solution, the specified assemblage is equilibrated with the first solution defined in the current simulation.

The **Save Solution as** allows you to save the composition of a simulation by creating a new equilibrium phase. These new 'elements' can then be used as input data for subsequent PHREEQC simulations. Each of these new elements must be identified by a unique number that is not already in use. If you specify a number that is currently in use, the new element will overwrite the old element.

7.3.3 Exchange Assemblage

Ion exchange involves the replacement of one chemical in the solution for another on a solid surface. Intrusion of fresh water into marine sediments or seawater into coastal fresh water aquifers are probably the most obvious examples for this mechanism. Fresh water typically is dominated by Ca2+ and HCO3- ions due to the presence of dissolved calcite, whereas in seawater, Na+ and Cl- are the dominant ions. Sediment in contact with sea water will often have large concentrations of Na+.

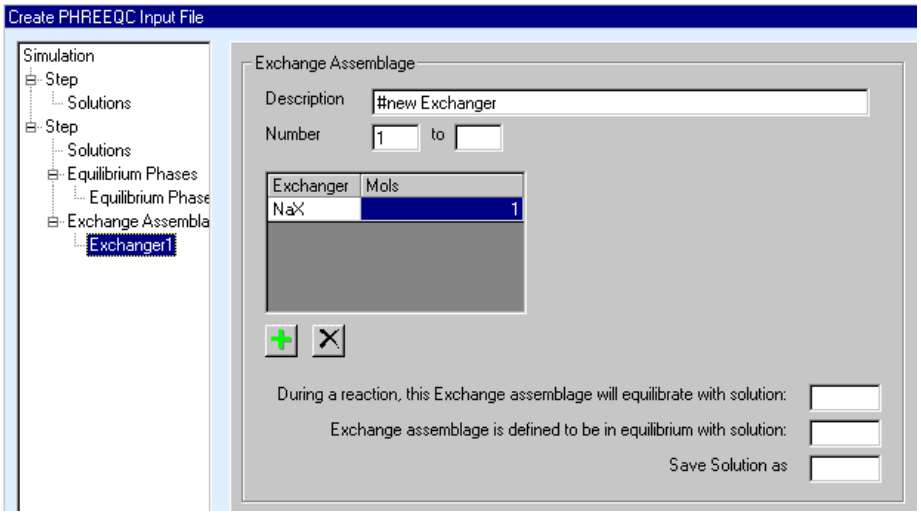
When seawater intrudes in a coastal fresh water aquifer an exchange of cations takes place:

$$2Na^+ + Ca\text{-}X_2 \rightarrow (2Na\text{-}X + Ca^{2+})$$

where X indicates the soil exchanger.

Sodium is taken up by the exchanger and Ca2+ is then released. The composition of the solution and the exchanger is modified by this reaction.

A sample of the **Exchange Assemblage** options dialogue is seen below:



PHREEQC lets you define the initial composition of an **Exchange Assemblage** in two ways:

1. Explicitly by selecting the composition of the Exchange Assemblage; or
2. Implicitly by specifying that the Exchange Assemblage is in equilibrium with a solution of a fixed composition.

Option 1

AquaChem provides a comprehensive list of available exchanger ions to choose from and allows you to easily add several ions to the Exchange Assemblage.

To add an ion(s) to the Exchange Assemblage:

- Click  to add a new line to the grid.
- Under the **Exchanger** field, double-click in the first empty cell and a combo box with a  button will appear listing the available items.
- Select the ion you need, and press **<Enter>** (on your keyboard). The ion will appear in the grid.
- Enter the Amount (in **Mols**) for each ion in the **Exchanger** column. In order to estimate the amount of exchangeable cations, you may use the Aquifer calculator.

To remove an ion from the Exchange Assemblage, click-on the ion you would like to remove, and then press the  button.

Option 2

You may specify that the Exchange assemblage is defined to be in equilibrium with a solution. Simply enter a solution number in the appropriate field.

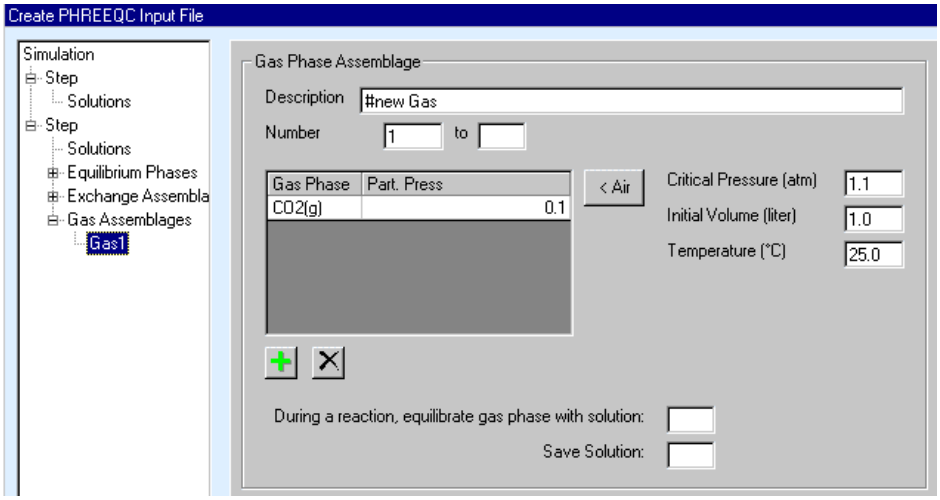
Once you have defined the Exchange Assemblage, you must select the solution with which you wish to equilibrate. If you do not select a solution from the list, you can save the Exchange Assemblage to equilibrate in a later simulation step (e.g. during a transport problem).

Each Exchange Assemblage is identified by a unique **Number** and a **Description** so they can be easily recognized in the Input / Output files, and reused in later simulations.

The **Save Solution as** field allows you to save the composition of a simulation by creating a new exchange assemblage. These new 'elements' can then be used as input data for subsequent PHREEQC simulations. Each of these new elements must be identified by a unique number that is not already in use. If you specify a number that is currently in use, the new element will overwrite the old element.

7.3.4 Gas Phase Assemblage

The Gas Phase is used to equilibrate a solution with a finite volume of gas. This simulation is not applicable if fixed partial pressures of the gas components are desired (for this case use the Mineral Phase option instead and fix a gas with a partial pressure that has an infinite volume of gas phase). An example of the **Gas Phase Assemblage** dialogue is shown below:



The Gas Phase option will equlibriate the solution with only those gases which are defined in the simulation. However, gases may be specified with a partial pressure equal to zero at the start of the simulation. In this case, no moles of that component will be present initially, but some gases may evolve during a reaction simulation such as

oxidation of organic material. As a result, the partial pressure of all gases included in the gas phase stays constant and the excess gas is removed from the solution as the gas bubbles.

Pressure calculations are computed using the ideal gas law,

$$PV=nRT$$

where,

P = defined pressure
V = volume
n = number of moles of the gas
R = universal gas constant
T = temperature

AquaChem provides a list of available gases to choose from and allows you to easily add multiple gases to the **Gas Phase Assemblage**.

To add a gas phase assemblage to the simulation:

- Click  to add a new line to the grid.
- Under the **Gas Phase** field, double-click in the first empty cell and a combo box with a  button will appear listing the available items.
- Select the gas you need, and press **<Enter>** (on your keyboard). The gas will appear in the grid.
- Enter a partial pressure value for each gas under the **Part. Press** column.

If you wish to add air to the solution, click on 

button and the major components of air will be automatically added to the list, with their partial pressures at 1 bar.

To remove a gas from the **Gas Phase Assemblage** table, select the gas to remove and then press the  button.

The **Critical Pressure**, **Initial Volume** and **Temperature** information is required for each Gas Phase assemblage in order to calculate the weights of each gas component.

The default values are:

Critical Pressure: **1.1** atm.
Initial Volume: **1.0** liters
Temperature: **25°**C

Finally, you can select the solution with which you would like to equilibrate the gas phase assemblage. If you do not select a solution from the list, you can save the gas

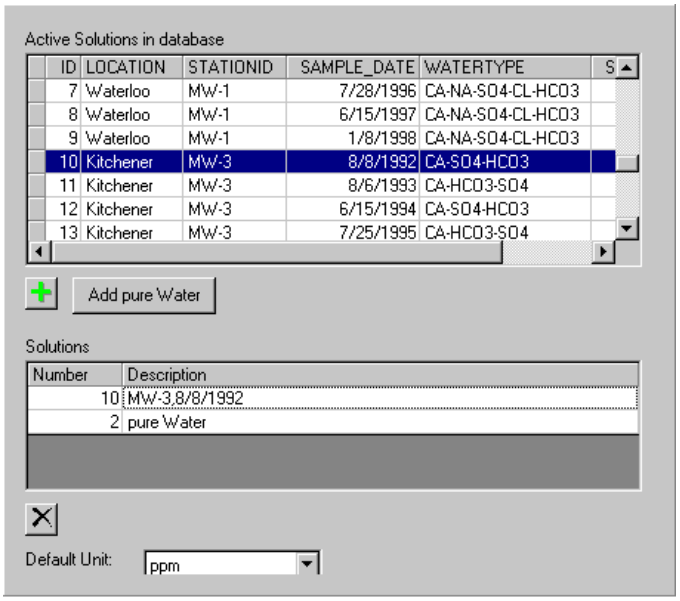
phase to equilibrate in a later simulation step. Each Gas Phase Assemblage is identified by a unique number and can be reused in later simulations.

The **Save Solution as** allows you to save the composition of a simulation by creating a new gas phase assemblage. These new 'elements' can then be used as input data for subsequent PHREEQC simulations. Each of these new elements must be identified by a unique number that is not already in use. If you specify a number that is currently in use, the new element will overwrite the old element.

7.3.5 Adding Solutions

In PHREEQC, a "solution" is a set of analyses for a single water sample. AquaChem automatically creates a PHREEQC input file from the sample details pertaining to your AquaChem database, or from a pure water sample.

To access the solutions options, expand the items in the **Navigator tree** by pressing the **+** beside **Step**. Then select **Solutions** and the solutions frame should appear, similar to the one below.



You must specify at least one solution for every PHREEQC simulation file. AquaChem allows you to select from two types of solutions:

- Samples from your AquaChem database; OR
- Pure Water

These options are described in detail in the following sections.

Using Samples from your AquaChem Database

To add a sample from your database as a solution, select the sample from the list at the top, and press the  button. The sample will then be added to the **Solutions** frame in the lower half of the dialogue; in addition, the new solution will show up as a new line in the **Navigation tree**, under **Solutions**.

To add multiple samples from your database, use the **<Shift>** and **<Ctrl>** keys with the mouse to select the samples you need, then click the  button. This is useful if you want to speciate a large number of samples simultaneously. Each complete sample should have pH, alkalinity, and temperature values specified.

The AquaChem database index **Number** for the selected sample will be used as the Solution number. The **Description** field is used to identify the solutions. The solution description will appear in the PHREEQC input file.

After you have added a solution, you can verify that it has been added to the PHREEQC input file. To do so, click the **Input File** tab at the bottom of the screen and you should see the added solution and any corresponding concentrations.

Adding Pure Water

To add pure water as a solution, press the 

button below the list of AquaChem active solutions. For certain simulations it might be useful to have pure water as a base solution. For example, you can simulate a groundwater by saturating pure water with calcite and adding a specified CO2 pressure.

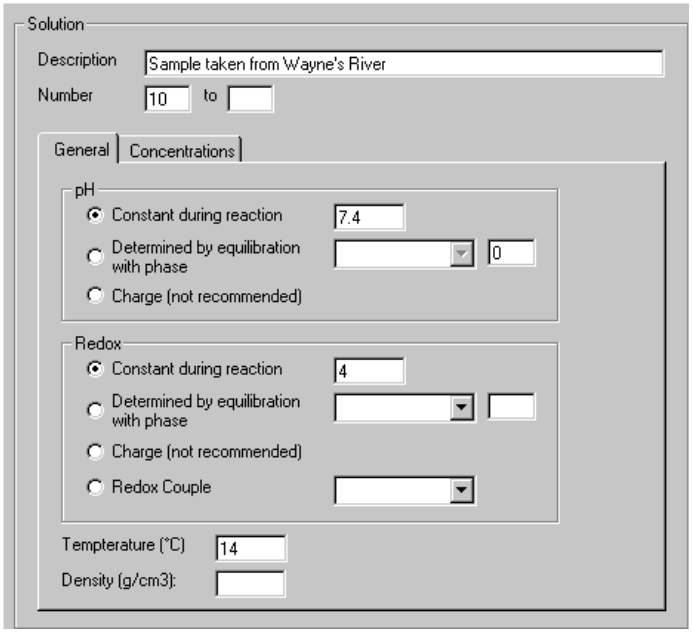
Solution Properties

Once you have added a solution, you may want to modify the Solution properties.

To do so, you have two options:

- In the **Solutions** frame, double click on the appropriate solution from the main dialogue, OR
- Select the appropriate **Solution #**, from the **Navigator tree** on the left side of your display.

The **Solutions** properties frame should appear as shown below.



The upper part of this dialogue lists the solution **Description** and **Number**. As discussed above, the **Number** is AquaChem database index number for the selected sample which will be used as the Solution number. The **Description** field is used to identify the solutions.

The remaining options in this frame are separated into two tabs:

- **General**, and
- **Concentrations**

The options associated with these tabs are described in detail in the following section.

General

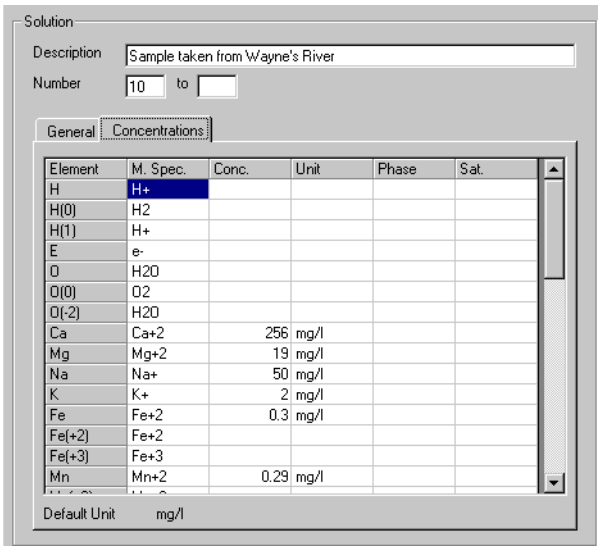
Under the **General** tab, you can specify options for **pH** and **Redox** during the simulation.

You can choose a **Constant during reaction** value for these parameters, or allow the values to be determined as a result of equilibration with a mineral phase (**Determined by equilibrium with phase**).

In addition, at the bottom of the frame, you can enter a default **Temperature** and **Density** values for the simulation.

Concentrations

This tab lists the concentrations of the dissolved elements in solution.



The first column of the grid contains the **Element** name, while the second column describes the PHREEQC Masterspecies (**M. Spec.**) name.

The parameter values are read from the database; if necessary you may add or remove concentrations (**Conc.**), or edit the existing values. You may also define a concentration as controlled by a mineral solubility, or for gases, by a defined pressure. For example, a calcium concentration is overridden in the simulation by a calculated value that will result in a calcite equilibrium state (Saturation index = 0).

Once you have entered element values for the pure water solution, the **Default Unit** may not be changed. However, you can change the unit individually for each entered value by clicking button in the **Unit** column. Please note that it is not possible to freely mix units (i.e. you may not enter some values as mg/L and others as mmol/l). You may only mix units within a "unit family" such as g/L, mg/L ug/L.

Example

The following example will demonstrate how to use a sample from the Demo database, as a solution in a PHREEQC simulation:

To add the **MW-1-92** sample from the **DEMO.AQC** database to a PHREEQC input file, proceed as follows:

- **Tools** from the main menu, then select **Modeling** and then **PHREEQC (Basic)** from the main menu.
- Click **+** beside **Step** (in the **Navigator tree**) and you will see **Solutions**
- Select **Solutions**
- Select the **MW-1-92** sample (ID = 1) at the top of the list of **Active solutions in database** frame
- Click  button and the sample will now appear in the **Solutions** frame in the bottom section of the dialogue.

To view the solution properties, double click on this **Solutions**, or expand the **Navigator tree**, and select the **Solution** from here. This will load a **Solution** properties dialogue.

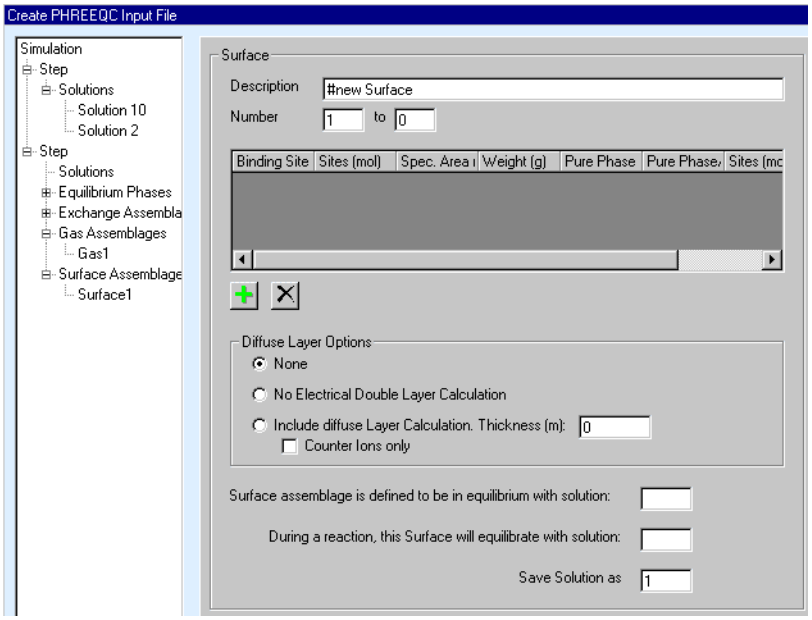
Click on the **Concentrations** tab to confirm that the concentrations are identical to those entered for that sample in the AquaChem database.

To verify that this data is saved to the PHREEQC input file, you can view the input file by clicking the **Input File** tab at the bottom of the dialogue.

7.3.6 Surface Assemblage

While ions are exchanged during an exchange process, surface processes involve only the absorption of material on mineral surfaces. This process typically can be observed on hydroxides and is driven by electrostatic processes.

An example of the **Surface** options dialogue is seen below:



PHREEQC lets you define the initial composition of a **Surface Assemblage** in two ways:

1. Explicitly by specifying the parameter values for Surface Assemblage; or
2. Implicitly by specifying that the Surface Assemblage is in equilibrium with a solution of a fixed composition.

Option 1

To define a Surface Assemblage:

- Click  to add a new line to the grid.
- Under the **Binding Site** field, double-click in the first empty cell and a combo box with a  button will appear listing the available items.
- Select a Binding site, and press **<Enter>** (on your keyboard).
- Type in default values for **Specific Area** (600 **m2**) and **Weight** (0 **g**)
- Specify the total number of **Sites** (in **mols**) for each binding and make any appropriate changes to the default values for **Specific Area** and **Weight**.
- Choose the appropriate diffuse layer model for the surface reaction (please see the PHREEQC manual for information on selecting the appropriate **Diffuse Layer Options** for your surface reactions).

To remove a binding site from the Surface Assemblage, select the **Binding Site** you would like to remove and press the  button.

Option 2

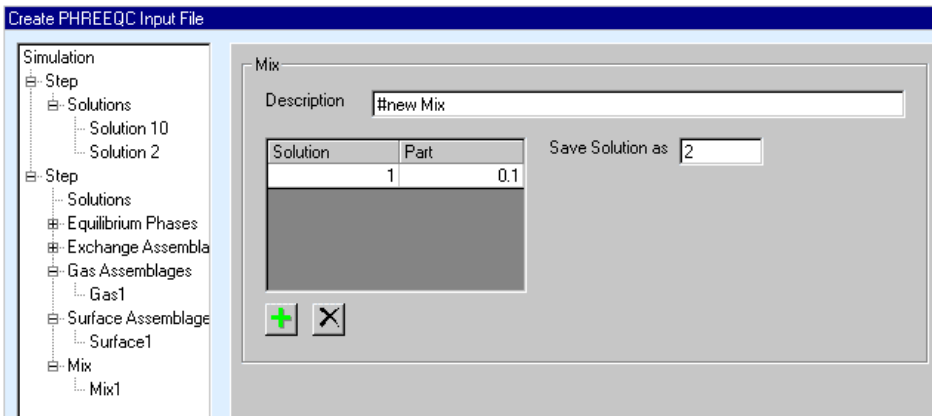
You may specify that the Surface assemblage is defined to be in equilibrium with a solution. Simply enter a solution number in the appropriate field.

Once you have defined the Surface Assemblage, you must select the solution with which you wish to equilibrate. Each Surface Assemblage is identified by a unique **Number** and a **Description** so they can be easily recognized and reused in later simulations.

The **Save Solution as** allows you to save the composition of a simulation by creating a new surface assemblage. These new 'elements' can then be used as input data for subsequent PHREEQC simulations. Each of these new elements must be identified by a unique number that is not already in use. If you specify a number that is currently in use, the new element will overwrite the old element.

7.3.7 Mix Solutions

The Mix Solutions allows you to simulate the mixing of multiple solutions together with different proportions of each solution added to the mixture. An example of the **Mix** options dialogue is seen below:



To simulate mixing multiple samples together, you must first specify at least two solutions for the PHREEQC simulation.

To add a solution to the mixture:

- Click  to add a new line to the grid under the **Solution** header.
- Type in a Solution number in the same cell.

- Click-on the first line in the grid under the **Part** header and type the proportion of the solution you would like to add to the mixture (e.g. 3 parts of Solution 1 and 4 parts of Solution 2)

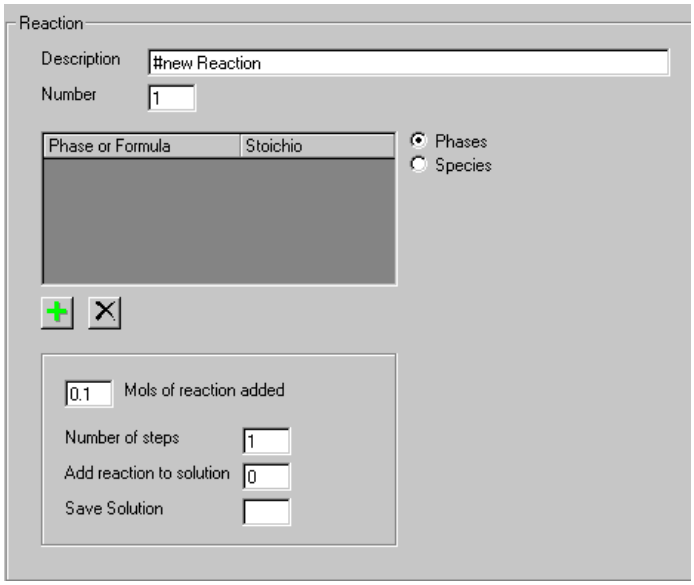
The solutions will be automatically added to the input file.

Each mixed solution has a unique Mix number and a **Description** and can be used in a later simulation. To re-use these, simply enter a solution number beside the **Save Solution as** field.

7.3.8 Reactions

The Reactions simulation options are used to dissolve or precipitate a specified amount of a mineral or to perform another chemical reaction. The Reactions dialogue allows you to specify multiple reactions for the simulation by giving each reaction a unique identification number and a text description.

To access these options, you need to add a **Reaction** as a **Step** and then access the **Reactions** options. Below is an example of the **Reaction** dialogue:



AquaChem provides a comprehensive list of available reactant species and phases to choose from. To select from the list of available reactants:

- Specify to show **Phases** or **Species**
- Click  to add a new Phase or Species. A new line will be added to the grid.

- Under the **Phase or Formula** field, double-click in the first empty cell and a combo box with a button will appear listing the available reactants.
- Select the reactant you need, and press **<Enter>** (on your keyboard). The reactant will appear in the grid.
- Enter the stoichiometric factor (SF) in the **Stoichio** field beside the reactant. The stoichiometric factor defines whether the reactants are added (SF>0) or removed (SF<0) from the solution. The stoichometric factor is the amount of a reactant relative to the other reactants (default value is **1**).
- Type the number of **Moles of reactant added**, the **Number of steps** for the reaction, and **Add reaction to solution** number. The reaction path is revealed when you simulate the reaction in multiple steps. By default the reaction is added to the first solution in the simulation. Note that you are not required to add the reaction immediately to a solution if you only wish to use the reaction in later simulation step(s).
- To add additional reactions, you must add additional Reaction steps. To do this, select **Reactions** from the **Navigator tree**. Then, under the **Reactions** frame, click to add a new Reaction. A new line will be added to the navigator tree. Select this new item, and the options will be loaded for this new reaction.

The **Save Solution as** allows you to save the composition of a simulation by creating a new reaction. These new 'elements' can then be used as input data for subsequent PHREEQC simulations. Each of these new elements must be identified by a unique number that is not already in use. If you specify a number that is currently in use, the new element will overwrite the old element.

The reaction will be added automatically to the input file. To verify this, click the **Input File** tab at the bottom of the dialogue.

NOTE: AquaChem is capable of recognizing species that are not available in the PHREEQC thermodynamic database. AquaChem will recognize the chemical composition of a given formula for reactions, if it is entered correctly in the phase field.

The following example demonstrates how to add a reaction.

Example

Follow the steps listed below to specify the following reaction:

Dissolve 0.1 moles **Calcite** and 2.0 moles **Halite** (NaCl) in pure water.

- Select **Tools** from the main menu, then **Modeling** and then **PHREEQC (Basic)** from the main menu.

The **PHREEQC Input** dialogue will appear, and the **General** tab will be active.

- Click **+** beside **Step** (in the **Navigator tree**) and you will see **Solutions**
- Select **Solutions**
- Add **pure water** as a solution by clicking 

below the active solutions frame
- Click **Step** from the **Navigator tree** and right click on it
- Select **Add Forward Model** and then select **Add Reaction** to add the First Reaction step.
- **Reactions** a new item **Reaction1** will now appear in the **Navigator tree**.

Under the **Reaction** options (in the **Navigator tree)**:

- Select **Reaction1** in the **Navigator tree**
- **Phase** radio button, under the **Reaction** options frame
- Click  to add a new Phase or Species. A new line will be added to the grid.
- Under the **Phase or Formula** field, double-click in the first empty cell and a combo box with a button will appear listing the available reactants.
- Select **Calcite**, a default value of **1.0** will show for calcite. Press **<Enter>** on your keyboard.
- type: **0.1** in the **Mols of reaction added** field (located below the grid)
- Select the field labeled **Add reaction to solution**.
- Type **1** in this field.

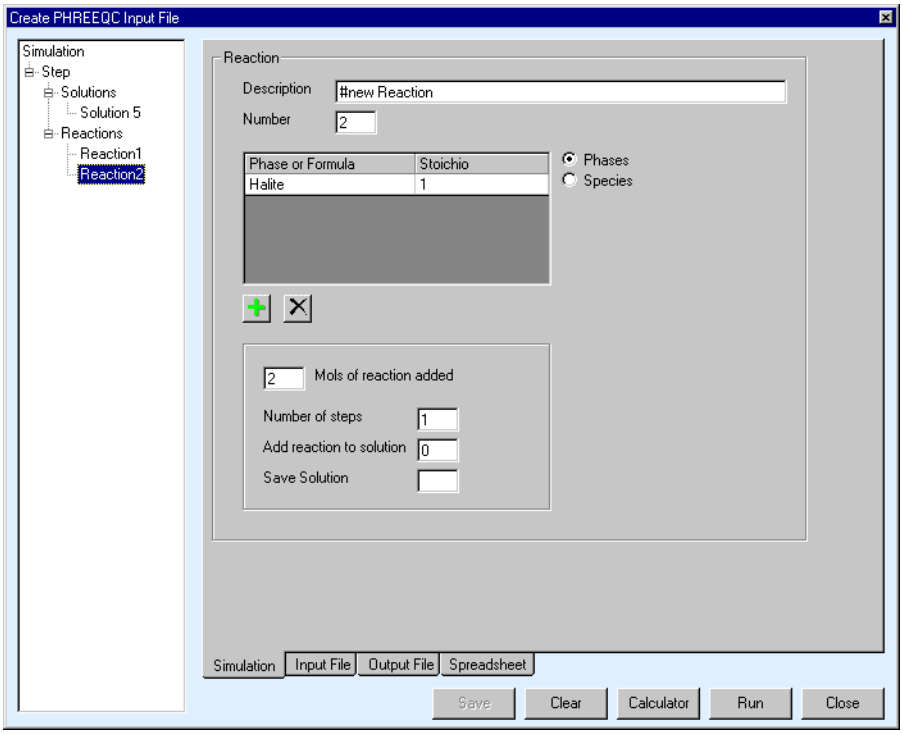
This reaction will be automatically added to the input file. To verify this, click the **Input File** tab at the bottom of the dialogue.

Repeat the above steps to add the Second Reaction step. Notice that the Reaction number has automatically incremented to '**2**".

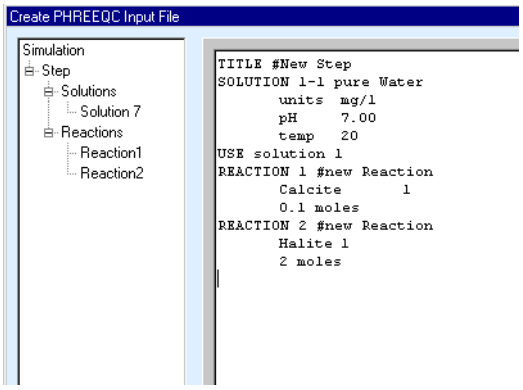
To add a reaction for **Halite**:

- **Reaction2** in the **Navigator tree**.
- Click  to add a new Phase or Species. A new line will be added to the grid.
- Under the **Phase or Formula** field, double-click in the first empty cell and a combo box with a button will appear listing the available reactants.
- Select **Halite**, and a default value of **1.0** will show. Press **<Enter>** on your keyboard.
- type: **2.0** in the **Mols of reaction added** field (located below the grid) for Halite.

Once you have added this reaction, your dialogue should appear similar to the one shown below:



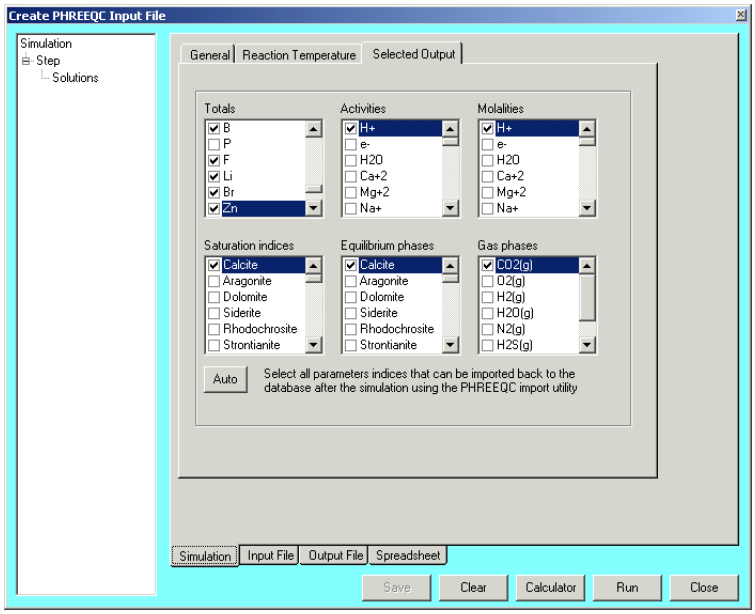
To verify the input file, click on the **Input File** tab at the bottom of this dialogue. The contents of the input file should be similar to that shown in the figure below:



You may now run PHREEQC with these reaction and solution options.

7.4 Running PHREEQC Simulation

Once you have specified the necessary Solutions and Reaction Steps, you are ready to run the simulation. Before doing so, it is recommended that you verify the contents of the input file. In addition, be sure to specify the output options under the **Selected Output** tab (as shown below).



Once this is finished, click the **[Run]** button to run the simulation.

The PHREEQC simulation will run in the background as a DOS application inside a DOS window. Once the simulation is finished, you can verify the results by clicking the **Output File** tab (at the bottom of the main PHREEQC dialogue) and scan this for any error messages.

7.5 Viewing PHREEQC Output

The output from the PHREEQC run can be viewed by clicking on the **Output File** tab, or on the **Spreadsheet** tab. The results may be copied back to your samples in your AquaChem database. Simply highlight the contents of the output file, and copy the contents to the clipboard (by pressing Ctrl-C). Then, you may paste the data into your AquaChem samples, by pressing Ctrl-V (you must first close the PHREEQC interface). After that, you may proceed to use the modeled data in plots, reports, and database queries.

References

Appelo, C.A.J. and Postma, D., 1993: *Geochemistry Groundwater and Pollution*. A.A. Balkeema. Rotterdam, 536 p.

Balderer, W., Pearson , F. J. jr., and Soreau, S., 1991: *Sulphur and Oxygen Isotopes in Sulfate and Sulfide*. In F. J. J. Pearson, W. Balderer, H. H. Loosli, B. E. Lehmann, A. Matter, T. Peters, H. Schmassmann, & A. Gautschi (Eds.), Applied Isotope Hydrogeology a case Study in northern Switzerland - NTB 88-01 Amsterdam - Oxford - New York - Tokyo: Elsevier.

Balderer, W., Pearson, F. J., Rauert, W., and Stichler, W., 1991: *Isotopic Composition of Groundwater.* In: F. J. Pearson, W. Balderer, H. H. Loosli, B. E. Lehmann, A. Matter, T. Peters, H. Schmassmann, & A. Gautschi (Eds.), Applied Isotope Hydrogeology - A Case Study In Northern Switzerland. - Studies in Environmental Science (pp. 98-115).

Drever, J. I., 1982: *The Geochemistry of Natural Waters*. Prentice Hall, New Jersey, Amsterdam: Elsevier, 437 p.

Fournier, R. O., 1981: *Application of Water Chemistry to Geothermal Exploration and Reservoir Engineering*. In: L. Rybach & L. J. P. Muffler (Eds.), Geothermal Systems: Principles and Case Histories, New York: Wiley, pp. 109-143.

Giggenbach, W.F., 1988. *Geothermal solute equilibria*. Derivation of Na-K-Mg-Ca geoindicators. Geochim Cosmochim. Acta, 52: pp. 2749-2765.

Giggenbach, W.F., 1989: *The chemical and isotopic position of Ohaaki field within the Taupo Volcanic Zone*. Proc. Eleventh N.Z. Geothermal Workshop, Aukland: pp. 81-88.

Hounslow, A.W. 1995: *Water Quality Data – Analysis and Interpretation*. CRC Press LLC. pp. 75-85.

Howard, P.H. et al. 1991: *Handbook of Environmental Degradation Rates*, Lewis Publishers, 775 p.

Kharaka, Y. K., Gunter, W. D., Affarwall, P. K., Perkins, E. H., and De Braal, J. D., 1988: *Solmineq.88: A computer Program Code for Geochemical Modelling of Water-Rock Interactions*. In U.S.Geological Survey Water Investigations Report 88-05.

Kharaka, Y. K., and Mariner, R. H., 1989: *Chemical Geothermometers and their Application to formation waters from sedimentary basins*. In: N. D. Näser & T. H. Lloyd, J. W., and Heathcote, J. A., 1985: *Natural inorganic hydrochemistry in relation to groundwater* - An Introduction. Oxford: Clarendon Press.

McCulloh (Eds.), Thermal History of Sedimentary Basins; Methods and Case Histories, Springer Verlag, pp. 99-117.

Nordstrom, D. K., Plummer, L. N., Langmuir, D., Busenberg, E., Man, H. M., Jones, B. F., and Parkhurst, D. L., 1990: *Revised Chemical Equilibrium Data for Major Water-Mineral Reactions and their Limitations*. In: D. C. Melchior & R. L. Bassett (Eds.), Chemical Modelling of Aqueous Systems Washington: American Chemical Society.

Parkhurst D.K., Thorenston D.C. and Plummer N.L., 1980: *PHREEQE - A computer program for geochemical calculations*. U.S. Geological Survey Water Resource Investigations 80-96, 210 p. http://gwrp.cciw.ca/gwrp/software/software.html

Pearson, F. J. J., Lolcama, J. L., and Scholtis, A., 1989: *Chemistry of Waters in the Böttstein*, Weiach, Riniken, Schafisheim, Kaisten and Leuggern Boreholes: A Hydrochemically consistent Data Set. No. NTB 86-19, Nagra.

ReedM.and Spycher N., 1984: *Calculations of pH and mineral equilibria in hydrothermal waters with application to geothermy and studies of boiling and dilution.* Geochimica and Cosmochimica Acta, 48, pp. 1479-1492.

Stumm, W., and Morgan, J. J., 1981: *Aquatic chemistry* (2^{nd} ed.). New York: John Wiley & Sons.

Tukey J.W., 1977: *Exploratory Data Analysis*, Addison-Wesley, Reading, Massachusetts, USA. pp. 39-43.

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Troubleshooting and Frequently Asked Questions

The following list provides answers to some of the most common problems encountered by users of AquaChem. Please review this list of frequently asked questions before contacting WHI Technical Support for assistance with your project.

Q 1: *My sample symbols do not show up on the plot.*

A1. Check that you have assigned symbols to that sample(s).

A2. Ensure the symbol group is active for the plots. This can be set in the **Plots > Define Symbol or Line** dialogue.

A3. Ensure that you have entered data for each parameter required by that plot.

Q 2: *My symbols show up on the plot colored in red, even though I have assigned another color to this symbol*.

A. The red colored symbols correspond to the samples which are selected in the active list. This indicates you are using the **Identify Samples** option in the **Define Symbol or Line** dialogue. Disable this option and the symbols will no longer be identified.

Q 3. *After I import data, the data does not appear correctly or does not appear at all.*

A1. Check that you have a value for each sample for each parameter in your source file.

A2. Ensure that you have selected the correct **Delimiter** during the import routine.

A3. Check your data source file to ensure that there are no extra spaces between columns or rows of data.

Q 4: *During data import, I get an error "***Column must be assigned to CAS Registry #.***"*

A1. Ensure that you have specified the correct import format. For this warning, you should typically try the **Samples as Rows** in the **Format** field.

A2. If your data source file does not contain CAS Registry #'s, ensure that this option is disabled during the data import.

Q 5: *During data import, I get error "***Column must be assigned to SampleID or StationID***."*

A1. Ensure that you have specified the correct import format. For this warning, you should typically try the **Samples as Rows** in the **Format** field.

A2. Ensure that you have mapped at least one of your text fields as the StationID and SampleID.

Q 6: *Some of my samples or stations no longer appear in the active list.*

A. Since samples and stations are actively linked in the database, when you temporarily omit a station, the corresponding samples will be removed from the active list. Likewise, when you remove all samples assigned to a given station, this station will be temporarily removed from the active list. To restore all samples or stations press the **Show all** button in the active samples list dialogue, or select **Filter** from the main menu and then **Show all** option.

Q 7: *In the print options window, part of the plot is cut off by the print template.*

A. Be sure to select the print template first, then load the plot on top of the template. This will ensure the page margins are set correctly, and will not cut off sections of the plot.

Q 8: *After I enter a value for a measured parameter, the 0 after the decimal place is cut off (for example, 7.20 in entered, however AquaChem displays this as 7.2).*

A. This can be corrected by modifying the parameter format. Go to File > Database > Parameters. Select the appropriate measured parameter, and modify the format. Disable the Auto option, and increase the number of decimal places to the desired value.

Q 7: *Is it possible to create two unique Piper plots showing two different sample groups?*

A. AquaChem will not allow for multiple Piper plot windows showing two distinct sample groups, at the same time. Since plots are created from information based on the active samples list, any changes that are made in the active list will immediately impact any open plot windows. The plots must be created individually.

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